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NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom  
IPC display formats  
NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental  
spectra  
NEWS 16 MAR 31 CA/Caplus and CASREACT patent number format for U.S.  
applications updated  
NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI  
NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements  
NEWS 19 APR 04 STN AnaVist, Version 1, to be discontinued  
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predefined hit display formats  
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NEWS 22 APR 28 IMSRESEARCH reloaded with enhancements  
NEWS 23 MAY 30 INPAFAMDB now available on STN for patent family  
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NEWS 24 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology  
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NEWS 26 JUN 06 KOREAPAT updated with 41,000 documents  
  
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AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008  
  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

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COST IN U.S. DOLLARS                SINCE FILE          TOTAL
                                     ENTRY          SESSION
FULL ESTIMATED COST                0.21              0.21

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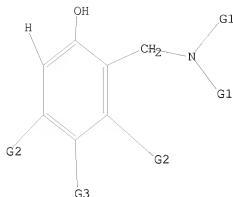
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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=> d l1
L1 HAS NO ANSWERS
L1 STR
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G1 H, Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu

G2 Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu

G3 H, Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, CF3, CC13, Cl, Br, F, I

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:54:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 653 TO ITERATE

100.0% PROCESSED 653 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 11527 TO 14593

PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> search l1

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full

FULL SEARCH INITIATED 14:54:13 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 12686 TO ITERATE

100.0% PROCESSED 12686 ITERATIONS

72 ANSWERS

SEARCH TIME: 00.00.01

L3 72 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

181.58

181.79

FILE 'CAPLUS' ENTERED AT 14:54:18 ON 09 JUN 2008

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=> s l3

L4 37 L3

=> d l4 fbib ab hitstr 1-37

L4 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:440649 CAPLUS

DN 148:402897

TI Long chain phenols. Part 42a. Phenolic structure and color in Mannich reaction products

AU Tyman, John H. P.; Patel, Mahesh

CS Department of Chemistry, Brunel University, Uxbridge, Middlesex, UB8 3PH, UK

SO Journal of Chemical Research (2007), (1), 34-37

CODEN: JCROA4

PB Science Reviews

DT Journal

LA English

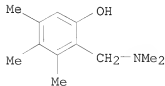
AB Mannich reactions were carried out with a variety of model alkylphenols and Me<sub>2</sub>NH, MeNH<sub>2</sub>, and HN[(CH<sub>2</sub>)<sub>2</sub>NH<sub>2</sub>]<sub>2</sub> to trace the origin of persistent colored products occurring in related reactions with pentadeca(e)nylphenol and 4-tert-alkylphenols. It was found to be attributable to the presence of resorcinolic impurities.

IT 89240-10-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(phenolic structure and color in Mannich reaction products)

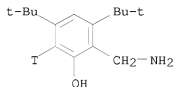
RN 89240-10-8 CAPLUS

CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



RE.CNT 30      THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 2004:859383 CAPLUS  
DN 142:373475  
TI Transition metal catalyzed sodium borotritide reductions: a useful  
alternative to the use of tritium gas  
AU Tang, Yui S.; Liu, Wensheng; Chaudhary, Ashok; Melillo, David G.; Dean,  
Dennis C.  
CS Merck Research Laboratories, Rahway, NJ, 07065, USA  
SO Synthesis and Applications of Isotopically Labelled Compounds, Proceedings  
of the International Symposium, 8th, Boston, MA, United States, June 1-5,  
2003 (2004), Meeting Date 2003, 71-74. Editor(s): Dean, Dennis C.; Filer,  
Crist N.; McCarthy, Keith E. Publisher: John Wiley & Sons Ltd.,  
Chichester, UK.  
CODEN: 69FZAZ; ISBN: 0-470-86365-X  
DT Conference  
LA English  
OS CASREACT 142:373475  
AB Sodium borotritide can be used in combination with transition metal  
additives for reduction of aryl halides and olefins as an alternative to  
traditional catalytic tritium gas reduction. This methodol. produces high  
specific activity product, demonstrates excellent chemoselectivity, and  
eliminates undesired tritium exchange.  
IT 849367-52-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(chemoselective preparation of tritium labeled arenes via reductive  
dehalogenation of arylhalides with sodium borotritide and palladium  
acetate)  
RN 849367-52-8 CAPLUS  
CN Phen-2-t-ol, 6-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX  
NAME)



RE.CNT 3      THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 2004:2832 CAPLUS  
DN 140:59400  
TI Preparation of aminoalkylphenols as antimalarials active against  
drug-resistant Plasmodia.  
IN Dorn, Conrad P.; Powles, Mary Ann; Walsh, Thomas F.; Wyvratt, Matthew J.  
PA Merck & Co., Inc., USA  
SO PCT Int. Appl., 51 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004000783	A1	20031231	WO 2003-US19393	20030620
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2490243	A1	20031231	US 2002-391361P CA 2003-2490243 US 2002-391361P WO 2003-US19393	P 20020624 20030620 P 20020624 W 20030620
	AU 2003251574	A1	20040106	AU 2003-251574 US 2002-391361P WO 2003-US19393	20030620 P 20020624 W 20030620
	EP 1517879	A1	20050330	EP 2003-761147 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK	20030620 P 20020624 W 20030620
	JP 2005534676	T	20051117	JP 2004-515965 US 2002-391361P WO 2003-US19393	20030620 P 20020624 W 20030620
	US 20050234265	A1	20051020	US 2004-511661 US 2002-391361P WO 2003-US19393	20041018 P 20020624 W 20030620
OS	MARPAT 140:59400				
AB	Title compds. [I; R5, R1a, R1 = H, alkyl, halo, alkoxy, cycloalkyl, aryl, trihalovinyl, said aryl optionally substituted with 1-3 R <sub>a</sub> ; R2 = H, alkyl, C3-10 cycloalkyl; taken together with any intervening atoms can form a 3-7 membered carbocyclyl, heterocyclyl unsatd., said heterocyclic ring containing 1-2 O, CO, S, SO, SO2, N, NR2a and optionally substituted by 1-3 R <sub>a</sub> ; R2a = H, alkyl; R3, R3a = H, halo, alkyl, C3-10 cycloalkyl, aryl, said aryl and alkyl optionally substituted with 1-3 R <sub>a</sub> ; R3R3a = atoms to form a 3-7 membered carbocyclyl, heterocyclyl saturated or unsatd., said heterocyclic ring containing 1-2 O, CO, S, SO, SO2, N, NR2a and optionally substituted by 1-3 R <sub>a</sub> ; R4 = H, halo, alkyl, trihaloalkyl; R <sub>a</sub> = alkoxy, alkyl, CF <sub>3</sub> , NO <sub>2</sub> , amino, cyano, alkylamino, halo; n = 1-3], were prepared. Thus, 3-tert-butylphenol and N-hydroxymethyl-2-chloroacetamide were added in portions to a vigorously stirred solution of AcOH and H <sub>2</sub> SO <sub>4</sub> at 0°; the reaction mixture was allowed to warm to room temperature over several hours,				
and	stirring was maintained for a total of 20 h to give a product which was heated in aqueous HCl at 85° for 3 h to give 2-aminomethyl-5-tert-butylphenol hydrochloride. I inhibited Plasmodium falciparum with IC <sub>50</sub> <1 µg/mL.				
IT	51571-04-1P 84210-35-5P 639069-27-5P 639069-29-7P 639069-31-1P 639069-33-3P 639069-34-4P 639069-35-5P 639069-36-6P 639069-37-7P 639069-38-8P 639069-39-9P 639069-40-2P 639069-41-3P 639069-42-4P 639069-49-1P 639069-58-2P 639069-59-3P 639069-60-6P 639069-62-8P 639069-64-0P				

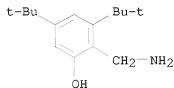
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 639069-78-6P 639069-79-7P 639069-80-0P  
 639069-83-3P 639069-88-8P 639069-90-2P  
 639069-92-4P 639070-01-2P 639070-04-5P  
 639070-05-6P 639070-06-7P 639070-08-9P  
 639070-64-7P 639070-65-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminoalkylphenols as antimalarials active against drug-resistant Plasmodia)

RN 51571-04-1 CAPLUS

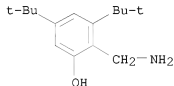
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI)  
 (CA INDEX NAME)



● HCl

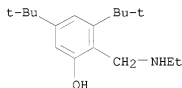
RN 84210-35-5 CAPLUS

CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



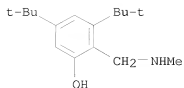
RN 639069-27-5 CAPLUS

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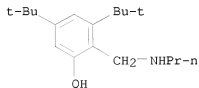


RN 639069-29-7 CAPLUS

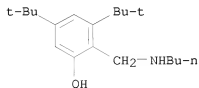
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(methylamino)methyl]- (CA INDEX NAME)



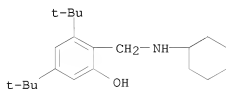
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 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(propylamino)methyl]- (CA INDEX NAME)



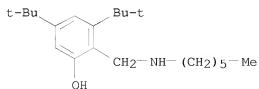
RN 639069-33-3 CAPLUS  
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RN 639069-34-4 CAPLUS  
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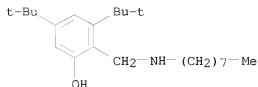


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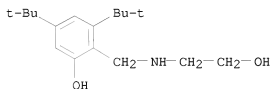




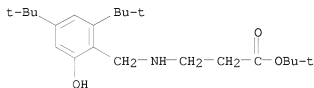
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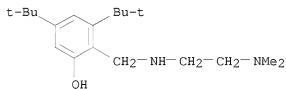
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 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[2-(2-hydroxyethyl)amino]methyl]- (CA INDEX NAME)



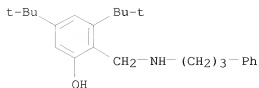
RN 639069-38-8 CAPLUS  
 CN β-Alanine, N-[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



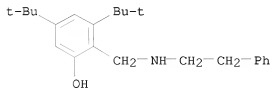
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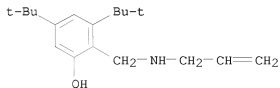
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 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[3-phenylpropyl]amino]methyl]- (CA INDEX NAME)



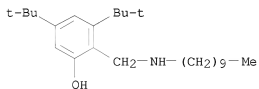
RN 639069-41-3 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(2-phenylethyl)amino]methyl- (CA INDEX NAME)



RN 639069-42-4 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(2-propen-1-ylamino)methyl]- (CA INDEX NAME)

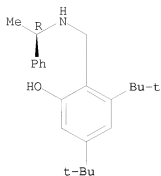


RN 639069-49-1 CAPLUS  
 CN Phenol, 2-[(decylamino)methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



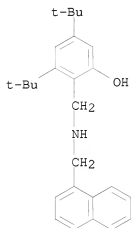
RN 639069-58-2 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(1R)-1-phenylethyl]amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



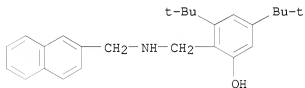
RN 639069-59-3 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[{(1-naphthalenylmethyl)amino)methyl]-  
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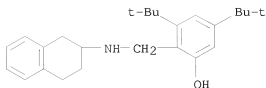
RN 639069-60-6 CAPLUS

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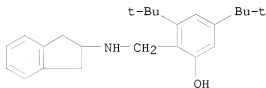
RN 639069-62-8 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[{(1,2,3,4-tetrahydro-2-naphthalenyl)amino)methyl]- (CA INDEX NAME)



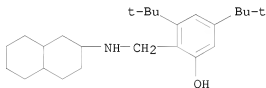
RN 639069-64-0 CAPLUS

CN Phenol, 2-[(2,3-dihydro-1H-inden-2-yl)amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



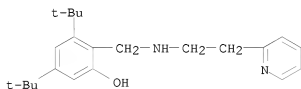
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CN Phenol, 2-[(decahydro-2-naphthalenyl)amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



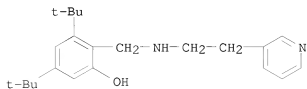
RN 639069-76-4 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(2-pyridinyl)ethyl]amino]methyl]- (CA INDEX NAME)

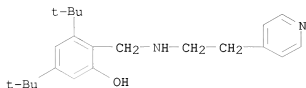


RN 639069-77-5 CAPLUS

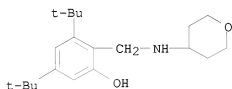
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(3-pyridinyl)ethyl]amino]methyl]- (CA INDEX NAME)



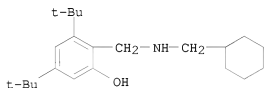
RN 639069-78-6 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(4-pyridinyl)ethyl]amino]methyl]-  
 (CA INDEX NAME)



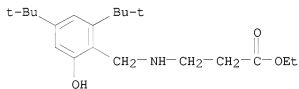
RN 639069-79-7 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(tetrahydro-2H-pyran-4-yl)amino]methyl]- (CA INDEX NAME)



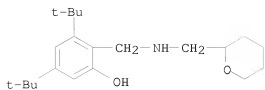
RN 639069-80-0 CAPLUS  
 CN Phenol, 2-[[[(cyclohexylmethyl)amino]methyl]-3,5-bis(1,1-dimethylethyl)-  
 (CA INDEX NAME)



RN 639069-83-3 CAPLUS  
 CN β-Alanine, N-[[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl]methyl]-,  
 ethyl ester (CA INDEX NAME)

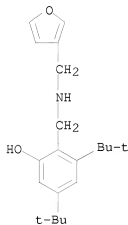


RN 639069-88-8 CAPLUS  
 CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[2-(tetrahydro-2H-pyran-2-yl)methyl]amino]methyl]- (CA INDEX NAME)



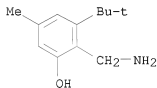
RN 639069-90-2 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[(3-furanylmethyl)amino]methyl]-  
(CA INDEX NAME)



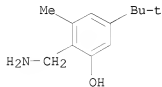
RN 639069-92-4 CAPLUS

CN Phenol, 2-(aminomethyl)-3-(1,1-dimethylethyl)-5-methyl]- (CA INDEX NAME)



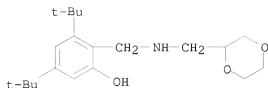
RN 639070-01-2 CAPLUS

CN Phenol, 2-(aminomethyl)-3-(1,1-dimethylethyl)-5-methyl]- (CA INDEX NAME)



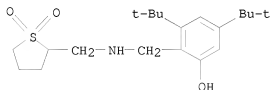
RN 639070-04-5 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[1,4-dioxan-2-ylmethyl)amino]methyl]- (CA INDEX NAME)



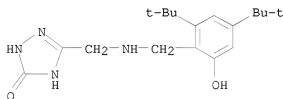
RN 639070-05-6 CAPLUS

CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(tetrahydro-1,1-dioxido-2-thienyl)methyl]amino]methyl]- (CA INDEX NAME)



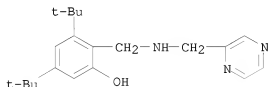
RN 639070-06-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[[[2,4-bis(1,1-dimethylethyl)-6-hydroxyphenyl)methyl]amino]methyl]-1,2-dihydro- (CA INDEX NAME)



RN 639070-08-9 CAPLUS

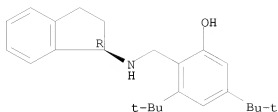
CN Phenol, 3,5-bis(1,1-dimethylethyl)-2-[[[(2-pyrazinylmethyl)amino]methyl]- (CA INDEX NAME)



RN 639070-64-7 CAPLUS

CN Phenol, 2-[[[[(1R)-2,3-dihydro-1H-inden-1-yl]amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

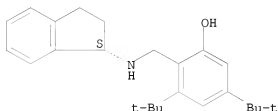
Absolute stereochemistry.



RN 639070-65-8 CAPLUS

CN Phenol, 2-[[[(1S)-2,3-dihydro-1H-inden-1-yl]amino]methyl]-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:857716 CAPLUS

DN 138:197738

TI A structurally characterized monomeric Mn(IV) complex in a discrete N2O4 coordination environment

AU Rajendiran, T. M.; Kampf, Jeff W.; Pecoraro, Vincent L.

CS Department of Chemistry, The University of Michigan, Ann Arbor, MI, 48109-1055, USA

SO Inorganica Chimica Acta (2002), 339, 497-502

CODEN: ICHAA3; ISSN: 0020-1693

PB Elsevier Science B.V.

DT Journal

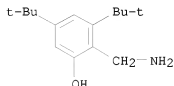
LA English

OS CASREACT 138:197738

AB From the reaction of Mn(III)(OAc)3 with (3,5-di-tert-butyl-2-hydroxyphenylmethyliminomethyl)3,5-di-tert-butyl-phenol (H2dbpip) in MeCN, dark brown crystals of compound Bis[(3,5-di-tert-butyl-2-hydroxyphenylmethyliminomethyl)3,5-di-tert-butylphenolato]manganese (IV), Mn(IV)(dbpip)2 (1) were obtained upon slow evaporation of the solvent. The structural assignments of 1, that were made in part by elemental anal. and magnetic susceptibility, were confirmed by single crystal x-ray diffraction studies which revealed that compound 1 crystallizes in the monoclinic, space group C2/c with a cell dimensions a = 49.746(8), b = 12.682(2), c 19.497(3) Å, α 90, β 94.240(3), γ 90°. Cyclic voltammetry reveals a quasi reversible redox wave corresponding to the Mn(III)/Mn(IV) couple. The EPR spectrum at 4 K consists of strong and weak signals near g = 2 and 4, resp. A comparison of the EPR spectrum to there obtained for other Mn(IV)N2O4 complexes reveals that 1 is a rare example of an axial Mn(IV) species with

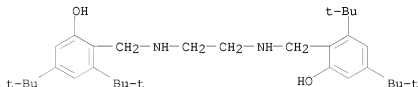


D $\alpha$ hv.  
 IT 84210-35-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of hydroxyphenylmethyliminomethylphenol)  
 RN 84210-35-5 CAPLUS  
 CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)

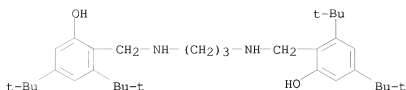


RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 2001:615153 CAPLUS  
 DN 136:5753  
 TI Single-step synthesis of salans and substituted salans by Mannich condensation  
 AU Tshuva, E. Y.; Gendeziuk, N.; Kol, M.  
 CS Raymond and Beverly Sackler Faculty of Exact Sciences, School of Chemistry, Tel Aviv University, Tel Aviv-Jaffa, 69978, Israel  
 SO Tetrahedron Letters (2001), 42(36), 6405-6407  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 136:5753  
 AB A convenient route for the synthesis of a variety of salan-type compds. is introduced. The synthesis is based on a single-step Mannich condensation between readily available starting materials: primary or secondary amines, formaldehyde and substituted phenols. This methodol. is suitable for the preparation of chiral salans as well, which may find applications in asym. catalysis.  
 IT 375793-66-1P 375793-68-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of salans by Mannich condensation)  
 RN 375793-66-1 CAPLUS  
 CN Phenol, 2,2'-[1,2-ethanediyldis(iminomethylene)]bis-3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 375793-68-3 CAPLUS  
 CN Phenol, 2,2'-[1,3-propanediyldis(iminomethylene)]bis[3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 1994:508209 CAPLUS  
DN 121:108209  
OREF 121:19519a,19522a  
TI Preparation of o-(aminoalkyl)phenols  
IN Ezaki, Yoichiro  
PA Arakawa Chem Ind, Japan  
SO Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAF

DT Patent  
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05331114	A	19931214	JP 1992-164390 JP 1992-164390	19920529 19920529

OS CASREACT 121:108209

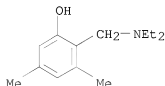
AB The title compds. are prepared by reaction of phenols having  $\geq 1$  unsubstituted o-position, aldehydes or ketones, and secondary amines followed by removing impurities from the reaction mixts. by treatment with alkali metal and/or alkaline earth metal hydroxides. A mixture of aqueous

Me<sub>2</sub>NH, 3,5-dimethylphenol, and aqueous HCHO was kept at 25-35° for 4 h, mixed with toluene, and the organic layer was treated with aqueous NaOH to give 86% 2-(N,N-dimethylaminomethyl)-3,5-dimethylphenol.

IT 38942-39-1P, 2-(N,N-Diethylaminomethyl)-3,5-dimethylphenol  
63487-28-5P, 2-(N,N-Dimethylaminomethyl)-3,5-dimethylphenol  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation from phenol and purification of)

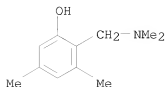
RN 38942-39-1 CAPLUS

CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)

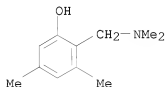


RN 63487-28-5 CAPLUS

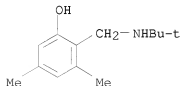
CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1991:562575 CAPLUS  
 DN 115:162575  
 OREF 115:27783a,27786a  
 TI Influence of structure and other characteristics of substitute fuel  
 components in petrol on engine efficiency and pollution  
 AU Stournas, S.; Lois, E.; Polyssis, P.; Serdari, A.; Swithenbank, J.;  
 Priestman, G. H.; Papachristos, M.  
 CS Fuels Lubr. Lab., Natl. Tech. Univ., Athens, 106 82, Greece  
 SO Comm. Eur. Communities, [Rep.] EUR (1991), EUR 13157, 157pp.  
 CODEN: CECED9; ISSN: 0303-755X  
 DT Report  
 LA English  
 AB Terpenic derivs., a new class of compds., Mannich base phenols, and  
 tertiary polyamines (>60 compds.) were evaluated for their antiknock  
 properties for 4 model gasolines. The effects of these additives on NOx,  
 CO, and HCHO emissions from a test engine were also determined  
 IT 63487-28-5 136029-09-9  
 RL: USES (Uses)  
 (gasoline antiknock additive, mol. structure effect and air pollution  
 in relation to)  
 RN 63487-28-5 CAPLUS  
 CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



RN 136029-09-9 CAPLUS  
 CN Phenol, 2-[(1,1-dimethylethyl)amino]methyl]-3,5-dimethyl- (CA INDEX  
 NAME)



L4 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1988:140707 CAPLUS

DN 108:140707  
 OREF 108:22935a,22938a  
 TI Triboelectrifying material for charging electrostatographic toner  
 IN Fukumoto, Hiroshi; Tanaka, Katsuhiko; Kawagishi, Yoji  
 PA Canon K. K., Japan; Orient Chemical Industries, Ltd.  
 SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61160763	A	19860721	JP 1985-819	19850109
	JP 06046314	B	19940615		
				JP 1985-819	19850109

AB The triboelectrifying material has on its surface a metal-salicylamine or alkylsalicylamine complex. The complex may be coated on carrier particles, on a developing sleeve, or on a developing doctor blade. An Fe powder may be coated with Co-salicylamine complex to give the title material. The material shows improved durability in providing images with constant d.

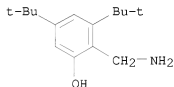
IT 84210-35-5D, complexes with transition metals

RL: USES (Uses)

(triboelectrifying agents, for electrostatog. toners, with improved durability)

RN 84210-35-5 CAPLUS

CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



L4 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:487767 CAPLUS

DN 103:87767

OREF 103:14097a,14100a

TI Cyclohexane-1,3-dione derivatives and their herbicidal compositions and methods

IN Serban, Alexander; Watson, Keith G.; Bird, Graham J.; Farquharson, Graeme J.

PA ICI Australia Ltd., Australia

SO U.S., 21 pp.

CODEN: USXXAM

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4511391	A	19850416	US 1983-497683	19830524
				AU 1983-4118	A 19830524

OS MARPAT 103:87767

AB Benzofuranilycyclohexenones and related compds. I [R = halo, NO2, cyano,

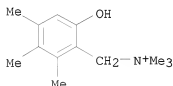
OH, (un)substituted alkyl, alkoxy, HO3SNH, etc.; R1 = (un)substituted alkyl, alkenyl, alkynyl; R2 = Ph, alkyl, furoalkyl, alkenyl, alkynyl; R3 = H, halo, cyano, alkyl, alkoxy carbonyl; R4 = H, (un)substituted alkyl, alkenyl, alkynyl, alkylsulfonyl, PhSO2, Bz, inorg. or organic cation; X, X1 = O, S, CH2; at least one of X and X1 is O or S; n = 1-3; n1 = 0-3] were prepared. Thus, phenol II (R5 = H) was treated with CH2O and HNMe2 to give II (R5 = CH2NMe2), which was quaternized with MeI and treated with Me2S(O):CH2 to give benzofuran III (R6 = H). III (R6 = H) was carboxylated and condensed with acetone to give III (R6 = CH:CH2COMe), which underwent cyclocondensation with (EtO2C)2CH2 to form cyclohexenylbenzofuran IV (R7 = H). IV (R7 = H) was acylated with (PrCO)2O to give IV (R7 = COPr), which condensed with EtONH2 to give IV (R7 = CPr:NOEt) (V). At 0.02 kg/ha postemergence, V inflicted 81-99% damage on Echinochola crus-galli, whereas winter wheat and rice were undamaged.

IT 89240-11-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of, benzofuran by)

RN 89240-11-9 CAPLUS

CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)



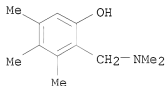
● I<sup>-</sup>

IT 89240-10-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and quaternization of)

RN 89240-10-8 CAPLUS

CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



L4 ANSWER 10 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:37229 CAPLUS

DN 102:37229

OREF 102:5799a,5802a

TI The crystal structures of 4,4'-bipyridinium  $\mu$ -(4,4'-

bipyridine)bis[diaquatetranitratoneodymate(III)]-tris(4,4'-bipyridine) and a second monoclinic form of triaquatrinitratoholmium(III)-bis(4,4'-bipyridine)

AU Weakley, Timothy J. R.

CS Dep. Chem., Dundee Univ., Dundee, DD1 4HN, UK

SO Inorganica Chimica Acta (1984), 95(6), 317-22

CODEN: ICHAA3; ISSN: 0020-1693

DT Journal

LA English

AB The 1st title compound is monoclinic, space group P21/c, with a 18.723(10), b 10.720(6), c 18.027(10) Å, and  $\beta$  94.43(5)°; Z = 2; R = 0.066 for 4931 data. The 2nd title monoclinic form has space group P21/c, with a 15.830(10), b 21.44(3), c 15.70(3) Å, and  $\beta$  100.4(2)°, Z = 8; R = 0.091 for 2335 film data. In the 1st compound pairs of Nd atoms are bridged across a crystal inversion center by a 4-bipy ligand, and 10-coordination is completed by 4 monodentate NO3, 3 bidentate NO3, and 2 H2O ligands, with bond lengths Nd-N 2.70, Nd-OH2(average) 2.44, and Nd-O(NO3, average) 2.56 Å. The 2nd compound has a variant of the previously-reported monoclinic [Y(NO3)3(H2O)3].2(4-bipy) structure, with doubling of the unit cell on a but with essentially no change in the geometry and orientation of the 9-coordinate complex. In both compds. the noncoordinated, nonprotonated 4-bipy N atoms form H bonds with ligand H2O.

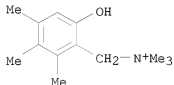
IT 89240-11-9

RL: PRP (Properties)

(structure of)

RN 89240-11-9 CAPLUS

CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

L4 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:121043 CAPLUS

DN 100:121043

OREF 100:18425a,18428a

TI Herbicidal cyclohexane-1,3-dione derivatives

IN Serban, Alexander; Watson, Keith Geoffrey; Bird, Graham John; Farquharson, Graeme John

PA ICI Australia Ltd., Australia

SO Eur. Pat. Appl., 86 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 95330	A1	19831130	EP 1983-302861	19830519
	EP 95330	B1	19871119		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AU 8314477	A	19831201	AU 1982-4118	A 19820524
	AU 560842	B2	19870416	AU 1983-14477	19830511
	ZA 8303398	A	19840229	AU 1982-4118	A 19820524
				ZA 1983-3398	19830511
	AT 30913	T	19871215	AU 1982-4118	A 19820524
				AT 1983-302861	19830519
				AU 1982-4118	A 19820524
				EP 1983-302861	A 19830519
	HU 31922	A2	19840628	HU 1983-1783	19830520
	HU 189285	B	19860630		
				AU 1982-4118	A 19820524
	JP 58213769	A	19831212	JP 1983-89300	19830523
	JP 05026788	B	19930419		
	CA 1202634	A1	19860401	AU 1982-4118	A 19820524
				CA 1983-428746	19830524
				AU 1982-4118	A 19820524

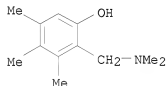
OS MARPAT 100:121043

AB Cyclohexanediones I [R = H, (un)substituted alkyl, Ph, SO<sub>3</sub>H, SO<sub>2</sub>Ph; R<sub>1</sub> = alkyl, fluoroalkyl, alkenyl, alkynyl, Ph; R<sub>2</sub> = (un)substituted alkyl, Ph; R<sub>3</sub> = H, halogen, cyano, alkyl, alkoxy carbonyl; R<sub>4</sub> = substituted Ph] were prepared. Thus, piperonal was treated with Me<sub>2</sub>CO and CH<sub>2</sub>(CO<sub>2</sub>Et)<sub>2</sub> to give II (R<sub>5</sub> = H) which was acylated with (EtCO)<sub>2</sub>O and treated with EtONH<sub>2</sub>.HCl to give II (R<sub>5</sub> = C<sub>6</sub>H<sub>5</sub>:NOEt)(III). At 0.2 kg/ha pre-emergence III gave 100% kill of Echinochloa crus-galli.

IT 89240-10-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and quaternization of)

RN 89240-10-8 CAPLUS

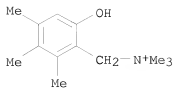
CN Phenol, 2-[(dimethylamino)methyl]-3,4,5-trimethyl- (CA INDEX NAME)



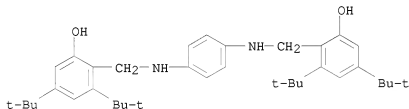
IT 89240-11-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with dimethylsulfoxium methylide)

RN 89240-11-9 CAPLUS

CN Benzenemethanaminium, 6-hydroxy-N,N,N,2,3,4-hexamethyl-, iodide (9CI) (CA INDEX NAME)



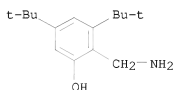
L4 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1983:163553 CAPLUS  
 DN 98:163553  
 OREF 98:24795a,24798a  
 TI Study of the effectiveness of inhibitors in oxidation of jet fuel in a closed volume  
 AU Kovalev, G. I.; Denisov, E. T.; Nikonova, A. G.; Gerasimova, A. V.; Burachevskaya, I. I.  
 CS Otd. Inst. Khim. Fiz., Chernogolovka, USSR  
 SO Deposited Doc. (1981), VINITI 443-82, 23 pp. Avail.: VINITI  
 DT Report  
 LA Russian  
 AB Extensive tests were conducted to study the antioxidative and heat stabilizing activity of amines, alkylphenols, aminophenols, and organophosphorus and organosulfur compds. in T6 jet aircraft fuel. The most effective were aminophenols. At 0.003 weight% concentration their ability to suppress the autoxidn. of T 6 at 170° exceeded the ability of Ionol [128-37-0]. The best antioxidant in this series was 4-phenylaminophenol [122-37-2].  
 IT 85404-01-9  
 RL: USES (Uses)  
 (antioxidants-heat stabilizers, for jet aircraft fuels)  
 RN 85404-01-9 CAPLUS  
 CN Phenol, 2,2'-[1,4-phenylenebis(iminomethylene)]bis[3,5-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1983:53306 CAPLUS  
 DN 98:53306  
 OREF 98:8181a,8184a  
 TI The use of sterically hindered benzylamines in the Sommelet reaction  
 AU Stokker, G. E.; Schultz, E. M.



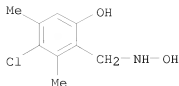
CS Merck Sharp Dohme Res. Lab., West Point, PA, 19486, USA  
 SO Synthetic Communications (1982), 12(11), 847-53  
 CODEN: SYNCAV; ISSN: 0039-7911  
 DT Journal  
 LA English  
 OS CASREACT 98:53306  
 AB Amines I (R = H, Me; R1 = H, halo, Me; R2 = H, alkyl, OMe; R3 = alkyl, H, Cl; R4 = H, alkyl, Cl, OMe) were converted to the resp. aldehydes II. Thus, I (R = R2 = R4 = H, R1 = iodo, R3 = CMe3) hydrochloride was heated with hexamethylenetetramine in aqueous HOAc to give II.  
 IT 84210-35-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Sommelet reaction of)  
 RN 84210-35-5 CAPLUS  
 CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)- (CA INDEX NAME)



L4 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1982:142446 CAPLUS  
 DN 96:142446  
 OREF 96:23413a,23416a  
 TI 2-Hydroxylaminomethyl phenols  
 IN Haviv, Fortuna  
 PA Abbott Laboratories, USA  
 SO U.S., 5 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

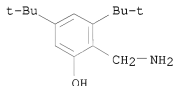
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	US 4312887	A	19820126	US 1978-954699	19781025
				US 1978-954699	A 19781025

OS CASREACT 96:142446; MARPAT 96:142446  
 AB Salicylaldehydes were converted to phenols I (R and R2 are H, alkyl, alkoxy, Cl; R1 = Cl, alkyl, alkoxy; R3 = H, halo, alkyl, alkoxy, alkylthio, CF3), which exhibited diuretic and antiinflammatory activity. Thus, 3,5-Cl(Me3C)C6H3CHO was oxidized and the oxime product was reduced by NaB(CN)H3 to give I (R1 = CMe3, R3 = Cl, R = R2 = H).  
 IT 81322-69-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation and diuretic activity of)  
 RN 81322-69-2 CAPLUS  
 CN Phenol, 4-chloro-2-[(hydroxyamino)methyl]-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



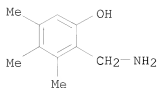
● HCl

L4 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1980:620454 CAPLUS  
 DN 93:220454  
 OREF 93:35187a,35190a  
 TI 2-(Aminomethyl)phenols, a new class of saluretic agents. 1. Effects of nuclear substitution  
 AU Stokker, G. E.; Deana, A. A.; DeSolms, S. J.; Schultz, E. M.; Smith, R. L.; Cragoe, E. J., Jr.; Baer, J. E.; Ludden, C. T.; Russo, H. F.; et al.  
 CS Merck Inst. Ther. Res., West Point, PA, 19486, USA  
 SO Journal of Medicinal Chemistry (1980), 23(12), 1414-27  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 OS CASREACT 93:220454  
 AB A series of .apprx.100 2-(aminomethyl)phenols was synthesized and tested in rats and dogs for saluretic and diuretic activity; several were highly active on i.v. or oral administration. The most active were 4-alkyl-6-halo derivs., especially 2-(aminomethyl)-4-(1,1-dimethylethyl)-6-iodophenol (I). I also had significant antihypertensive, topical saluretic, and antiinflammatory activity.  
 IT 51571-04-1P 51571-09-6P 75551-86-9P  
 75552-02-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as potential diuretic or saluretic agent)  
 RN 51571-04-1 CAPLUS  
 CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI)  
 (CA INDEX NAME)



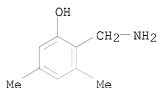
● HCl

RN 51571-09-6 CAPLUS  
 CN Phenol, 2-(aminomethyl)-3,4,5-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



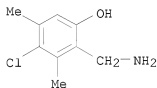
● HCl

RN 75551-86-9 CAPLUS  
 CN Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride (6CI, 9CI) (CA INDEX NAME)



● HCl

RN 75552-02-2 CAPLUS  
 CN Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

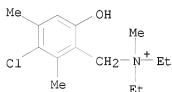


● HCl

L4 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1980:76524 CAPLUS  
 DN 92:76524  
 OREF 92:12611a,12614a  
 TI 3,4-Dihydro-2H-1,3-benzoxazin-2-one derivatives  
 IN Arct, Jacek; Jakubska, Elzbieta; Olszewska, Grazyna  
 PA Politechnika Warszawska, Pol.  
 SO Pol., 3 pp.  
 CODEN: POXXA7  
 DT Patent

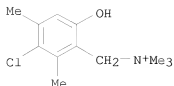
LA Polish  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	PL 100342	B1	19780930	PL 1975-185918 PL 1975-185918 A	19751223 19751223
AB	I [R, R1, R2 (same or different) = H, Cl, C1-5 alkyl, aryl, alkoxy, NO2, cyano, sulfonamido] were prepared by heating II [R3-5 (same or different) = C1-4 alkyl, X = Cl, alkyl or aryl sulfate, or 2-sulfonate] with an alkali cyanide at 70-140° 15-60 h in a polar solvent (MeNO2, MeCN, MeCOEt, DMF). Thus, 0.1 Mol KCN was added to 0.1 Mol III in 300 cc MeNO2, and the mixture refluxed 35 h to give 63% IV.				
IT	72724-29-9 RL: RCT (Reactant); RACT (Reactant or reagent) (ring closure of, with sodium cyanide)				
RN	72724-29-9 CAPLUS				
CN	Benzenemethanaminium, 3-chloro-N,N-diethyl-6-hydroxy-N,2,4-trimethyl-, chloride (9CI) (CA INDEX NAME)				

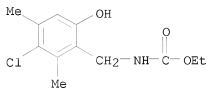


● Cl<sup>-</sup>

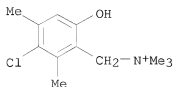
L4 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 1978:509299 CAPLUS  
DN 89:109299  
OREF 89:16837a,16840a  
TI Conversion of Mannich phenol bases; III. Synthesis and transformations of 3,4-dihydro-2H-1,3-benzoxazin-2-one derivatives  
AU Arct, J.; Jakubska, E.; Olszewska, G.  
CS Inst. Org. Chem. Technol., Warsaw Tech. Univ., Warsaw, Pol.  
SO Synthetic Communications (1978), 8(3), 143-9  
CODEN: SYNCAV; ISSN: 0039-7911  
DT Journal  
LA English  
OS CASREACT 89:109299  
AB Phenols I (R1, R2 = H, Me, Cl) cyclized with KO-CN to give 38-78% II, alcoholysis of which gave 86-99% III.  
IT 63616-12-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with cyanate, dihydrobenzoxazinone derivative from)  
RN 63616-12-6 CAPLUS  
CN Benzenemethanaminium, 3-chloro-6-hydroxy-N,N,2,4-pentamethyl- (CA INDEX NAME)



IT 67275-17-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 67275-17-6 CAPLUS  
 CN Carbamic acid, [(3-chloro-6-hydroxy-2,4-dimethylphenyl)methyl]-, ethyl  
 ester (9CI) (CA INDEX NAME)

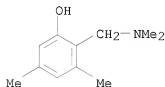


L4 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1977:484914 CAPLUS  
 DN 87:84914  
 OREF 87:13507a,13510a  
 TI Conversions of Mannich phenol bases; II. Synthesis of  
 2-thioxo-2H-3,4-dihydro-1,3-benzoxazine derivatives  
 AU Arct, Jacek; Jakubska, Elzbieta; Olszewska, Grazyna  
 CS Inst. Org. Chem. Technol., Warsaw Tech. Univ., Warsaw, Pol.  
 SO Synthesis (1977), (5), 314-15  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DT Journal  
 LA English  
 AB Benzoxazines I (R = 6-Me, 6-Cl, 6-Cl-7-Me, 5,7-Me2-6-Cl, 6,7-Cl2) were  
 prepared in 49-74% yield by reaction of the corresponding  
 o-hydroxybenzyltrimethylammonium salt with KSCN.  
 IT 63616-12-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with potassium thiocyanate)  
 RN 63616-12-6 CAPLUS  
 CN Benzenemethanaminium, 3-chloro-6-hydroxy-N,N,N,2,4-pentamethyl- (CA INDEX  
 NAME)



L4 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:468113 CAPLUS  
 DN 87:68113  
 OREF 87:10837a,10840a  
 TI Sulfones as chemical carriers of substances with germicidal activity.  
 VIII: Sulfonyl derivatives of the Mannich bases of quinaldine, pyrrole  
 and phenol  
 AU Messinger, Paul; Gompertz, Judith  
 CS Inst. Pharm. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.  
 SO Archiv der Pharmazie (Weinheim, Germany) (1977), 310(3), 249-55  
 CODEN: ARPMA5; ISSN: 0365-6233  
 DT Journal  
 LA German  
 OS CASREACT 87:68113  
 AB 4-MeC6H4SO2CH2CH2NMe2.HCl (R = 2-quinolyl) was prepared by treating  
 RCH2CH2NMe2 with 4-MeC6H4SO2H and aminomethylating RCH2CH2SO2C6H4Me-4. I  
 (NR1R2 = NMe2, piperidino) were obtained by treating 2-dimethylaminomethyl-  
 1-methylpyrrole methiodide with NaSO2Ph and aminomethylating  
 1-methyl-2-phenylsulfonylmethylpyrrole. II (NR1R2 = NMe2, piperidino,  
 morpholino) were similarly obtained from 2,4,6-HO(Me)2C6H2CH2NMe2.MeI.  
 4-MeC6H4SO2CH(CH2Bz)C6H3(OH)CH2NMe2.HCl-4,3 was prepared by aminomethylating  
 BzCH:CHC6H4OH-4 and treating 2,4-HO(BzCH:CH)C6H3CH2NMe2.HCl with  
 4-MeC6H4SO2H. 4-MeC6H4SO2CHPhCH2COC6H3(OH)CH2NMe2.HCl-4,3 was similarly  
 obtained from PhCH:CHCOC6H4OH-4.  
 IT 63487-28-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with toluenesulfinate)  
 RN 63487-28-5 CAPLUS  
 CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1974:120533 CAPLUS  
 DN 80:120533  
 OREF 80:19395a,19398a  
 TI Treating edema and hypertension using certain 2-aminoethylphenols  
 IN Cragoe, Edward J., Jr.; Schultz, Everett M.  
 PA Merck and Co., Inc.  
 SO U.S., 9 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3794734	A	19740226	US 1971-120730	19710303
	US 3979361	A	19760907	US 1975-600990	19750801
				US 1971-120730	A2 19710303
				US 1974-444200	A2 19740220

US 4044153	A	19770823	US 1976-684138	19760507
			US 1971-120730	A2 19710303
			US 1974-444200	A2 19740220
			US 1975-600990	A1 19750801

PATENT FAMILY INFORMATION:

FAN 1977:29478

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3979361	A	19760907	US 1975-600990	19750801
				US 1971-120730	A2 19710303
				US 1974-444200	A2 19740220
	US 3794734	A	19740226	US 1971-120730	19710303
				A	
	US 4044153	A	19770823	US 1976-684138	19760507
				US 1971-120730	A2 19710303
				US 1974-444200	A2 19740220
				US 1975-600990	A1 19750801

FAN 1977:551847

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4044153	A	19770823	US 1976-684138	19760507
				US 1971-120730	A2 19710303
				US 1974-444200	A2 19740220
				US 1975-600990	A1 19750801
	US 3794734	A	19740226	US 1971-120730	19710303
				A	
	US 3979361	A	19760907	US 1975-600990	19750801
				US 1971-120730	A2 19710303
				US 1974-444200	A2 19740220

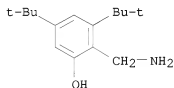
AB 2-(Aminomethyl)phenols (I; e.g., R = R2 = R3 = Cl, R1 = H; R = Me, R1 = R3 = H, R2 = Me3C; R = H, R1 = R3 = MeO, R2 = Cl), useful in the treatment of adema and hypertension, were prepared. Thus, treatment of 2,4,5-Cl3C6H2OH and ClCH2-CONHCH2OH with H2SO4 gave the amide (II) which, when treated with ethanolic HCl, gave I (R = R2 = R3 = Cl, R1 = H). About 24 I were prepared similarly.

IT 51571-04-1P 51571-09-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 51571-04-1 CAPLUS

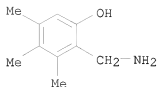
CN Phenol, 2-(aminomethyl)-3,5-bis(1,1-dimethylethyl)-, hydrochloride (9CI)  
(CA INDEX NAME)



● HCl

RN 51571-09-6 CAPLUS

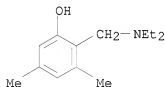
CN Phenol, 2-(aminomethyl)-3,4,5-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1972:514037 CAPLUS  
 DN 77:114037  
 OREF 77:18785a,18788a  
 TI Aminomethyl substituted phenol esters  
 IN Gablech, Miloslav; Major, Milan  
 SO Czech., 2 pp.  
 CODEN: CZXXA9  
 DT Patent  
 LA Czech  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CS 142844		19710915	CS 1968-8500	19681213
AB	<p>The title esters are prepared by esterification of phenols with acid anhydrides under conditions which prevent decomposition of the resulting Mannich bases. Thus, 2-[(diethylamino)methyl]-3,5-dimethylphenol, obtained by aminomethylation of m-xyleneol, was heated (1 mole) with 1.2 moles Ac2O 30 min at 50° with simultaneous in vacuo distillation of AcOH formed and excess Ac2O separated in vacuo to give 90% 2-[(diethylamino)methyl]-3,5-dimethylacetoxymethylbenzene.</p>				
IT	38942-39-1				
	<p>RL: RCT (Reactant); RACT (Reactant or reagent)          (acetylation of, with acetic anhydride)</p>				
RN	38942-39-1	CAPLUS			
CN	Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)				



L4 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1961:135955 CAPLUS  
 DN 55:135955  
 OREF 55:25561g-h  
 TI Diazo materials for prints  
 IN Slimowicz, Chester Edward



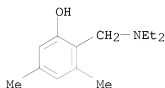
PA General Aniline & Film Corp.  
 DT Patent  
 LA Unavailable  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 867432		19610510	GB 1959-25553	19590724
	DE 1160732			DE	

AB A 2-component system of a light-sensitive diazo compound containing a Ph group substituted by a heterocyclic nitrogenous ring containing a hetero-O and a coupler compound, which is a derivative of a PhOH or resorcinol, produces prints

with little background discoloration. The usual S stabilizers are eliminated and storage with Ag van dyke prints is thus made practical. Cf. CA 37, 13425; 55, 2324d.

IT 38942-39-1  
 (Derived from data in the 6th Collective Formula Index (1957-1961))  
 RN 38942-39-1 CAPLUS  
 CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1961:135954 CAPLUS  
 DN 55:135954  
 OREF 55:25560a-4,25561a-g  
 TI Methine dyes  
 IN Ficken, Geoffrey Ernest; Kendall, John D.  
 PA Ilford Ltd.  
 DT Patent  
 LA Unavailable  
 FAN.CNT 1

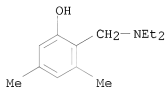
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 870753		19610621	GB 1957-21185	19570704

AB Cyanine dyes containing the 3,4-diazaindene ring system are useful as optical sensitizers in photographic Ag halide emulsions. Dyes were produced with the general formula A and B, where Z' is Q.N(R''').(CH:Z)n.C:CH(CH:CH)m or 4-AN(A'')C6H4CH:CH, A, A', R, R' are lower alkyl groups, R''' is a lower alkyl, hydroxyalkyl or aralkyl group, R'' is a lower alkyl or aralkyl group, n and m are 0 or 1, X' is Q'.C(:O).C:CHCH:, Z is CH or N, Q is the residue of a 5- or 6-membered heterocyclic ring, Q' is the residue of a keto-methylene nucleus, X is an acid radical, and Y is H or a lower alkyl. 2-Hydrazinopyridine (115 g.), 125 ml. iso-PrCOME and 300 ml. dry benzene were refluxed, the H2O formed removed by azeotropic distillation, the benzene distilled, and the residual oil heated with 1 g. ZnCl2 at 250° until NH3 evolution ceased, gave a product, b6 115°, which was redistd. The fraction b6 109-32° was extracted with ligroine (b. 60-80°) to give 1,1,2-trimethyl-3,4-diazaindene (I), m.p. 77-8° (cyclohexane). I (2.0 g.), 2.0 ml. MeI, and 10 ml. acetone

were refluxed for 0.5 hr. to give 1,1,2-trimethyl-3,4-diazaindene-4-MeI (II), m.p. 218-19° (decompose) (EtOH). 2-Methylthiobenzothiazole-MeI (III) (1.62 g.) and 1.52 g. II were refluxed in 30 ml. EtOH containing 1.0 ml. Et3N for 3 hrs. to give (1,1,4-trimethyl-3,4-diaza-2-indene) (3-methyl-2-benzothiazole)methinecyanine iodide, m. 313-14° (decompose) (MeOH) which extended the sensitivity of AgCl emulsions to 4950 Å., maximum 4700 Å. Similarly prepared were (4-ethyl-1,1-dimethyl-3,4-diaza-2-indene) (3-ethyl-2-benzothiazole)methinecyanine iodide, m. 318-19° (decomposition) (MeOH), and (1,1,4-trimethyl-3,4-diaza-2-indene) (1-methyl-2-quinoline)methinecyanine perchlorate, m. 250-1° (MeOH-HOCH2CH2OMe), both extending the sensitivity of AgCl from 4350 to 5800 Å. with maximum 5300 Å. 2-(2-Acetylanilinovinyl)benzoxazole-MeI (IV) (0.84 g.), 0.60 g. II and 5.0 ml. pyridine were refluxed for 0.25 hr. to give (1,1,4-trimethyl-3,4-diaza-2-indene) (3-methyl-2-benzoxazole)trimethinecyanine iodide, m. 268-9° (decompose) (MeOH-HOCH2CH2OMe), extending the sensitivity of Ag iodobromide to 6000 Å., maximum 5200 and 5600 Å. Similarly, (1,1,4-trimethyl-3,4-diaza-2-indene) (1,3,3-trimethyl-2-indolenine)trimethinecyanine perchlorate, m. 271-2° (decompose) (MeOH) was produced, extending the sensitivity of Ag iodobromide to 6250 Å., maximum 5900 and 6280 Å. HC(OEt)3 (1.6 ml.), 0.76 g. II, and 0.71 g. 3-methyl-1-phenyl-5-pyrazolone in 5 ml. pyridine were refluxed 0.5 hr. to give 4-(2,4-dihydro-1,1,4-trimethyl-3,4-diazainden-2-ylideneethylidene)-3-methyl-1-phenyl-5-pyrazolone, m. 251-2° (EtOH), extending sensitivity of AgCl emulsions from 4600-5550 Å., maximum 5350 Å. 5-Ethoxymethylene-3-ethyl-2-thio-4-thiazolidinone (V) (0.54 g.) and 0.76 g. II were refluxed in 10 ml. EtOH and 1.0 ml. Et3N for 20 min. to give 5-(2,4-dihydro-1,1,4-trimethyl-3,4-diazainden-2-ylideneethylidene)-3-ethyl-2-thio-4-thiazolidinone, m. 257-9° (MeOH-HOCH2CH2OMe), extending the sensitivity of Ag iodobromide to 6300 Å., maximum 6000 Å. p-Dimethylaminobenzaldehyde (0.30 g.) and 0.60 g. II were refluxed in 5 ml. pyridine containing 1 drop piperidine for 1.5 hr. to give 1,1-dimethyl-2-(p-dimethylaminostyryl)diazaindene-4-MeI, m. 272-3° (decompose) (MeOH), extending the sensitivity of Ag iodobromide to 6200 Å., maximum 5800 Å. 4-Methyl-2-methylthiothiazole-MeI and 0.79 g. II-EtI were refluxed in 10 ml. EtOH containing 0.5 ml. Et3N for 1 hr. and added to aqueous NaClO4 to give (4-ethyl-1,1-dimethyl-3,4-diaza-2-indene) (3,4-dimethyl-2-thiazole)methinecyanine perchlorate, m. 203-4° (EtOH), extending the range of AgCl from 4300 to 4750 Å., maximum 4600 Å. Similarly prepared was (4-ethyl-1,1-dimethyl-3,4-diaza-2-indene) (3-methyl-4-phenyl-2-thiazole)methinecyanine perchlorate, m. 289-90° (decompose) (MeOH), sensitivity of AgCl extended to 4850 Å., maximum 4650 Å. 2-(2-Ethylthiovinyl)quinoline-MeI (0.71 g.) and 0.60 g. II were refluxed in 10 ml. EtOH containing 0.5 ml. Et3N for 0.5 hr. to give (1,1,4-trimethyl-3,4-diaza-2-indene) (1-methyl-2-quinoline)trimethinecyanine iodide, m. 250-1° (decompose) (EtOH) and extended the sensitivity of Ag iodobromide from 5850 to 6550 Å. with maximum 6300 Å. Similarly produced were (1,1,4-trimethyl-3,4-diaza-2-indene) (1-methyl-4-quinoline)trimethinecyanine iodide, m. 298° (decompose) (MeOH); and (1,1,4-trimethyl-3,4-diaza-2-indene) (3-methyl-2-benzothiazole)trimethinecyanine iodide, m. 269-70° (MeOH), which extended the sensitivity of Ag iodobromide to 6400 Å., maximum 6050 Å. 1,1-Diethyl-2-methyl-3,4-diazaindene (VI) (0.66 g.) and 0.80 g. p-MeC6H4SO3Me (VII) were heated at 100° for 20 min., refluxed in 10 ml. pyridine with 1.1 g. IV for 1 hr., and poured into aqueous NaClO4. (1,1-diethyl-4-methyl-3,4-diaza-2-indene) (3-methyl-2-benzoxazole)trimethinecyanine perchlorate separated, m. 191° (EtOH). Similarly produced was (1,1-diethyl-4-methyl-3,4-diaza-2-indene) (3-methyl-2-benzothiazole)trimethinecyanine perchlorate, m. 203-3.5° (EtOH),

extending Ag iodobromide to 6250 A. with maximum 6000 A. A mixture of 0.70 g. VI, 0.70 g. 2-methylthioquinoline, and 1.6 g. VII was fused at 140° for 1.5 hr. and refluxed for 0.5 hr. with 5 ml. pyridine. Upon addition of aqueous NaClO<sub>4</sub>, (1,1-diethyl-4-methyl-3,4-diaza-2-indene)(1-methyl-2-quinoline)methinecyanine perchlorate precipitated, m. 207-8° (EtOH). A solution of 1.58 g. 1,1,2,5-tetramethyl-3,4-diazaindene-4-MeI (VIII) and 1.62 g. III in 20 ml. EtOH was refluxed with 1.0 ml. Et<sub>3</sub>N for 0.5 hr. (1,1,4,5-Tetramethyl-3,4-diaza-2-indene)(3-methyl-2-benzothiazole)methinecyanine iodide separated, m. 347-9° (decompose) (MeOH-HOCH<sub>2</sub>CH<sub>2</sub>OMe) and extended the sensitivity of AgCl to 5000 A. with maximum 4700 A. A mixture of 0.63 g. VIII and 0.54 g. IV was refluxed in 15 ml. pyridine for 0.5 hr. to give (1,1,4,5-tetramethyl-3,4-diaza-2-indene)(3-methyl-2-benzoxazole)trimethinecyanine iodide, m. 301-2° (decompose) (HOCH<sub>2</sub>CH<sub>2</sub>OMe); Ag iodobromide sensitivity was extended to 5800 A., maximum 5650 A. 1,1,2,7-Tetramethyl-3,4-diazaindene-4-MeI (IX) (0.63 g.) and 0.84 g. IV were refluxed in 5 ml. pyridine to give (1,1,4,7-tetramethyl-3,4-diaza-2-indene)(3-methyl-2-benzoxazole)trimethinecyanine iodide, m. 283-4° (MeOH) which extended Ag iodobromide sensitivity to 6050 A., maximum 5600 A. Similarly prepared was (1,1,4,7-tetramethyl-3,4-diaza-2-indene)(3-methyl-2-benzothiazole)trimethinecyanine iodide, m. 271-2° (MeOH) and extending Ag iodobromide sensitivity to 6400 A., maximum 5650 A., and 6000 A. A solution of 0.64 g. IX and 0.44 g. V in 10 ml. EtOH was refluxed with 0.5 ml. Et<sub>3</sub>N for 0.5 hr. to give 5-(2,4-dihydro-1,1,4,7-tetramethyl-3,4-diazainden-2-ylideneethylidene)3-ethyl-2-thio-4-thiazolidinone, m. 297-8° (decompose) (HOCH<sub>2</sub>CH<sub>2</sub>OMe), which extended the sensitivity of a Ag iodobromide emulsion to 6350 A. with maximum 5600 and 6000 A.

IT 38942-39-1, Phenol, 2-(diethylaminomethyl)-3,5-dimethyl-  
(in diazotype process)  
RN 38942-39-1 CAPLUS  
CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)

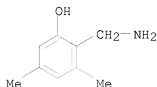


L4 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 1961:93325 CAPLUS  
DN 55:93325  
OREF 55:17572c-1,17573a-b  
TI Structure of synthetic resins. VIII. The preparation of 3,5-disubstituted 2-hydroxybenzaldehydes  
AU Zigeuner, G.; Jellinek, K.  
CS Univ. Graz, Austria  
SO Monatshefte fuer Chemie (1959), 90, 297-305  
CODEN: MOCMB7; ISSN: 0026-9247  
DT Journal  
LA Unavailable  
AB cf. CA 54, 8690f. The following (ArCH<sub>2</sub>)<sub>2</sub>NH (I) were prepared by heating the corresponding phenol with (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> (II) [Ar, reaction time (hrs.), reaction temperature, g. phenol, g. II, % yield, crystallization solvent, and m.p.

listed]: 5,2,3,6-Cl(OH)(Me2CH)2C6H (III), 2, 130°, 18.4, 15, 87, EtOH, 126°; 5,2,3,6-Br(OH)Me2C6H (IV), 2, 130°, 10, 7, 82, EtOH, 180°; 2,3,6-HO(Me2CH)MeC6H2 (V), 2, 125°, 6.15, 5.13, 68, EtOH, 100°; 2,5-HOMeC6H3 (VI), 3-4, 105°, 20, 2.6, -, xylene, 171°; 2,4,6-HOMe2C6H2 (VII), 3/4, 110°, 3, 1.2, -, EtOH, 181°; 2,3,6-HOMe2C6H2 (VIII), 2, 130°, 5, 11, 90, EtOH, 150°. Treatment of 4 g. 2,4,6-HOMe2C6H2CHO with 2 g. N2H4.H2O in EtOH produced the corresponding aldazine, m. 232° (alc.-H2O), 3 g. of which was reduced with 20 g. Zn powder in 260 mL. boiling EtOH and 30 mL. AcOH to VII. PhOH (10 g.), 4 g. H3BO3, and 5 g. II in 40 mL. (CH2OH)2 boiled 2 h., poured into H2O, the precipitate crystallized several times from dioxane gave a H3BO3 salt, m. 206-10°, saponified with 3 mL. concentrated HCl in 7 mL. EtOH, followed by NaOH, to I (Ar = o-HOC6H4), m. 161°. The following p-MeC6H4NHCH2Ar were prepared by heating the corresponding I 2 h. with p-toluidine (IX) (starting compound, reaction temperature, crystallization solvent, and m.p. listed): III, 120°, -, 110°; IV, 120°, cyclohexane, 137°; V, 160°, ligroine, 106°; VI, 160°, cyclohexane, 106°. A mixture of 4.7 g. 2,3,5-HOMe2C6H2CHO (X) and 6 g. 2,3,5-HOMe2C6H2CH2NH2.HCl, heated 1 h. with 2.5 g. NaHCO3 in 6 mL. EtOH, yielded 2,3,5-HOMe2C6H2CHNCH2C6H2Me2OH-3,5,2 (XI), m. 149° (MeOH); this compound heated 4 h. at 160° with IX formed 2,3,5-HOMe2C6H2CH2NHC6H4Me-p, m. 92°, and 2,3,5-HOMe2C6H2CH:NC6H4Me-p, m. 45° (MeOH); the latter compound was also obtained from IX and X at 180°. A mixture of 78 g. 3,5,4-Me2ClC6H2OH, 45 g. AcNH2, and 22.5 g. paraformaldehyde, saturated with HCl, gave after 3 days 5,2,4,6-Cl(OH)Me2C6H2CH2NHAC, m. 175° (EtOH), hydrogenated over Raney Ni to 2,4,6-HOMe2C6H2NHAC, m. 135° (C6H6); saponification of this compound by 8-h. reflux with 200 mL. concentrated HCl and 100 mL. EtOH yielded 2,4,6-HOMe2C6H2CH2NH2.HCl, m. 160° (decomposition) (AcOH), condensed with 2,4,6-HOMe2C6H2CHO (XII) in the presence of NaHCO3 to 2,4,6-HOMe2C6H2CH2N:CHC6H2Me2OH-4,6,2 (XIII), m. 203°; reduction over Pt gave VII. A mixture of 2 g. [2,3,5-HOMe2C6H2CH2]2NH (XIV), 6.2 g. m-O2NC6H4SO3Na (XV), and 3 g. NaOH in 10 mL. H2O boiled 2 h., acidified with H2SO4, and steam-distilled (method A) gave 1.10 g. 2,3,5-HOMe2C6H2CHO (XVI), m. 26° [oxime, m. 139° (petr. ether)], and 0.4 g. 2,3,5-HOMe2C6H2CO2H, m. 179°; 2 g. XIV, 6 g. XV, and 30 mL. AcOH refluxed 2 h. formed 1.6 g. XVI (method B); [2,3,5-HO(Cl)2C6H2CH2]2NH treated by A gave 55% 2,3,5-HOCl2C6H2CHO (XVII), m. 95° (oxime, m. 196°), and some 2,3,5-HOCl2C6H2CO2H, m. 224°, IV formed by A 36% 5,2,3,6-Br(OH)Me2C6H2CHO (XVIII), m. 87° (oxime, m. 181°), and some 5,2,3,6-Br(OH)Me2C6HCO2H, m. 239°; XVIII was obtained in 75% yield by B; III yielded 27% 5,2,3,6-Cl(OH)(Me2CH)MeC6HCHO (XIX), m. 59° (oxime m. 164°), by A, 71% by B; [4,3,5-HOMe2C6H2CH2]3N yielded by A 25% 4,3,5-HOMe2C6H2CHO, m. 115° (oxime, m. 190°), and some (4,3,5-HOMe2C6H2)2CO, m. 215°; VI gave 33% 2,5-HOMeC6H3CHO, m. 56°, by A, none by B; [2,5-HO(tert-Bu)C6H3CH2]3N gave 29% 2,5-HO(tert-Bu)C6H3CHO (XX) (oxime m. 113°) and some 2,5-HO(tert-Bu)C6H3CO2H, m. 151°, by A, nothing by B; VIII yielded 10% 2,3,6-HOMe2C6H2CHO by A, while VII formed only traces of an aldehyde; 2,6,3-[2,5-HO(tert-Bu)C6H3CH2NHCH2]2(tert-Bu)C6H2OH gave by A XX and 2,6,4-(CHO)2(tert-Bu)C6H2OH, m. 106° (oxime m. 113°); XI and XIII yielded by A XVI and XII, resp. A mixture of 5 g. 2,4-xyleneol and 16.5 g. II heated 3 h. at 140°, treated with 15 g. XV in 60 mL. AcOH, boiled 2 h., and steam-distilled gave 4.1 g. XVI; similarly, p-chlorothymol formed 78% XIX; 4,2,6-Br-Me2C6H2OH gave 75% XVIII; treatment of 2,4-Cl2C6H3OH with II, followed by reflux

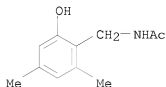
with NaOH and XV gave 55% XVII.

- IT 75551-86-9P, Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride  
99985-48-5P, Acetamide, N-(4,6-dimethylsalicyl)-  
100129-50-8P, Acetamide, N-(5-chloro-4,6-dimethylsalicyl)-  
109247-43-0P, Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl-  
RL: PREP (Preparation)  
(preparation of)  
RN 75551-86-9 CAPLUS  
CN Phenol, 2-(aminomethyl)-3,5-dimethyl-, hydrochloride (6CI, 9CI) (CA INDEX NAME)

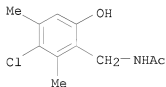


● HCl

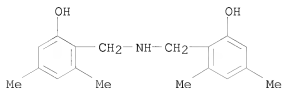
- RN 99985-48-5 CAPLUS  
CN Acetamide, N-(4,6-dimethylsalicyl)- (6CI) (CA INDEX NAME)



- RN 100129-50-8 CAPLUS  
CN Acetamide, N-(5-chloro-4,6-dimethylsalicyl)- (6CI) (CA INDEX NAME)

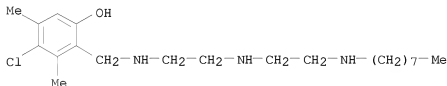


- RN 109247-43-0 CAPLUS  
CN Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1960:59461 CAPLUS  
 DN 54:59461  
 OREF 54:11521c-e  
 TI Amphoteric surface-active organic compounds  
 IN Schmitz, Adolf; Cramer, Gunter  
 PA Goldschmidt Akt.-Ges.  
 DT Patent  
 LA Unavailable  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2907791		19591006	US 1955-508768	19550516
AB	These compds. possessing germicidal and detergent properties may be prepared by causing to react at elevated temps. an amine, HCHO, and a phenol. Thus, PhOH 94, dodecyl-diethylenetriamine (I) 271, and 37% HCHO 81 parts were caused to react with considerable heat evolution. A light yellow sirup, 1-dodecyl-7-(x-hydroxybenzyl)diethylenetriamine, resulted. Similarly treated were: p-chloro-m-cresol, I, and HCHO; p-cresol, octyldiethylenetriamine (II), and HCHO; p-chloro-m-xylenol, II, and HCHO; phenol, 4-dodecylbenzyltriethylenetetramine, and HCHO; p-cresol, II (2 moles), and HCHO (2 moles); p-chloro-m-cresol, I (2 moles), and HCHO (2 moles); salicylic acid, I (2 moles), and HCHO (2 moles); p-hydroxybenzoic acid, I (2 moles), and HCHO (2 moles); 2,2-bis(4-hydroxyphenyl)propane, I (4 moles), and HCHO (4 moles). The salicylic acid derivative kills Micrococcus aureus (Staphylococcus aureus), Escherichia coli, and Bacterium proteus vulgaris (Proteus vulgaris) in a 1:8000 dilution in 10 min.				
IT	103508-55-0, Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (amphoteric germicidal surface-active)				
RN	103508-55-0 CAPLUS				
CN	Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)				

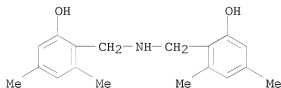


L4 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1960:22796 CAPLUS  
 DN 54:22796  
 OREF 54:442f-i, 4443a-h  
 TI The structure of artificial rosins. VII. Oxidative degradation of the methylene-nitrogen bridges in phenol-hexamethylenetetramine condensates  
 AU Zigeuner, G.; Jellinek, K.  
 CS Univ. Graz, Austria  
 SO Monatshfte fuer Chemie (1959), 90, 232-8  
 CODEN: MOCMB7; ISSN: 0026-9247  
 DT Journal  
 LA Unavailable  
 AB cf. C.A. 53, 15000h. Degradation via oxidative alkali melts gives insight

into the hardening of PhOH with (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>, e.g. bonding occurs mainly in the o-position of PhOH with formation of dibenzylamines and chains, while bonding in the p-position occurs only after prolonged heating and higher temps. 2,2'-Dihydroxy-3,3',5,5'-tetramethyldibenzylamine (I) and tris(2-hydroxy-3,5-dimethylbenzyl)amine (II) are easily converted to hydroxytrimesic acid (III) by use of an oxidative alkali melt with PbO<sub>2</sub> which rapidly degrades the CH<sub>2</sub>-N bridges, but under the same conditions 2,2'-dihydroxy-3,3',6,6'-tetramethylbenzylamine (IV) and 2,2'-dihydroxy-4,4',6,6'-tetramethylbenzylamine (V) undergo decarboxylation, IV to 2-hydroxyisophthalic acid (VI), and V to 2-hydroxyterephthalic acid (VII) and 5-hydroxyisophthalic acid (VIII). The degradation of xylenol-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> condensates IV and V via oxidative alkali melts proceeds along unknown paths and leads to products from whose constitution the structure of the starting materials cannot be determined with certainty, but the degradation of PhOH-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> condensates proceeds without side reaction, e.g. o-hydroxybenzylamine (IX) and 2,2'-dihydroxydibenzylamine (X) form salicylic acid (XI), 4-hydroxybenzylamine, 4,4'-dihydroxydibenzylamine, and the tribenzylamine (XII) yield p-hydroxybenzoic acid (XIII). The three-ring compds. 2,6-bis(2-hydroxybenzylaminomethyl)phenol (XIV) and 2,6-bis(4-hydroxybenzylaminomethyl)phenol (XV) are synthesized by dehalogenation of 2,6-bis(acetylaminomethyl)-4-chlorophenol (XVI) with Raney Ni to 2,6-bis(acetylaminomethyl)phenol (XVII), saponification of XVII to 2,6-bis(aminomethyl)phenol (XVIII), which with o-, and p-HOC<sub>6</sub>H<sub>4</sub>CHO, resp., forms the three-ring azomethine from which is formed XIV and XV by catalytic hydrogenation. Via oxidative alkali melts XIV is split into XI and VI, and XV into XI and VI. The separation of the acids is worked out preparatively, also the paper chromatography of the phenol carboxylic acids. The PhOH-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> rosins are prepared by hardening PhOH and (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> in 3:2 mole ratio at various temps, and reaction times. PhOH and (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>, on hardening at 100°, combine almost exclusively in the o-position with the formation of X and o-substituted chains of the type XIV. Only on oxidative degradation of rosins which are hardened longer at 100° and above can the formation of XVII be observed, which supposes the formation of p-compds. But here too, the o-compds. XI and VI constitute the main yield. Hardening at 180° of a condensate which forms at 100° by a three-dimensional bonding with NH<sub>3</sub> splitting off forms III through oxidative degradation. Through oxidative degradation are affected not only CH<sub>2</sub>-N bridges, but also CH<sub>2</sub> bridges. The PhOH-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> condensates obtained at 100-30° contain mainly CH<sub>2</sub>-N bridges, as shown by N values, while those obtained at 180° contain CH<sub>2</sub> bridges besides, although the position of the bridges cannot be determined by the results. PhOH-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> condensate (2 g.) is mixed intimately with 9-11 g. PbO<sub>2</sub> and introduced portionwise with good stirring into a melt of 40 g. KOH and 10 g. H<sub>2</sub>O at 320°, cooled, carefully diluted with 50 ml. H<sub>2</sub>O, acidified with 50% H<sub>2</sub>SO<sub>4</sub>, made alkaline, the precipitated PbSO<sub>4</sub> separated and washed well, the filtrate acidified again, extracted several times with ether, the ether dried, evaporated, and the residue treated with superheated steam to yield XI. The residue is extracted with hot H<sub>2</sub>O, VI crystallizing out of the filtrate. The residue contains XII. III is obtained by evaporating the aqueous phase after Et<sub>2</sub>O separation and extraction of the evaporated residue. Oxidation of I yields 76% III and of II, 75% III. Yields of VI from IV and VII and VIII from V are small. On paper chromatography the following results are obtained with S & S 2043a/gi, descending in 80:4:16 EtOH-concentrated aqueous NH<sub>3</sub>-H<sub>2</sub>O, 1% FeCl<sub>3</sub> solution as developer (acid, RF, color of spots, and

ultraviolet fluorescence given): XI, 0.75, blue, strongly blue; XIII, 0.57, weakly yellow, -; VII, 0.50, blue, strongly light blue; 4-hydroxyphthalic acid, 0.41, violet, weakly blue; VI, 0.31, pink, dark blue; VIII, 0.25, -, strongly yellow; III, 0.12, yellow-brown, blue. p-ClC6H4OH (60 g.) is dissolved in 150 ml. saturated alc. HCl and treated with methylolacetamide (from 70 g. AcNH2 and 35 g. paraformaldehyde), HCl gas added 24 hrs. under ice cooling, the precipitating XVI.HCl separated, taken up in H2O, and XVI liberated by dilute NH3 in 60% yield, m. 202° (40% EtOH). XVI (6 g.) in 100 ml. EtOH, 3 ml. H2O and 0.9 g. NaOH is hydrogenated in the presence of 10 g. Raney Ni till H absorption ceases, neutralized, the solvent evaporated in vacuo, and the residue recrystd. from H2O several times to yield XVII, prisms, m. 175°, yield 80%. Over 30 g. XVII is poured 50 ml. EtOH and 150 ml. HCl (d. 1.19), and with addition of HCl 6-8 hrs. refluxed, cooled, and saturated with HCl gas to precipitate XVIII.HCl, long spears, m. 215° (decomposition). XVIII.HCl (11.5 g.) is dissolved in 100 ml. EtOH, and boiled 30 min. with 12.5 g. o-HOC6H4CHO and 8.6 g. NaHCO3. On cooling, the azomethine (XIX), yellow needles, m. 187° (xylene), seps. XIX (2 g.) is dissolved in 50 ml. EtOH and 3 ml. HCl (d. 1.19) and hydrogenated with a PtO2 slurry (100 mg. PtO2 in 20 ml. EtOH). Evaporation yields hygroscopic crystals of XIV.HCl, from which is obtained XIV (decomposition from 180°) through NaHCO3 treatment. In the same manner XV is obtained by treatment of XVIII with p-HOC6H4CHO and NaHCO3 to form the azomethine, weakly yellow needles, m. 183°, which is then reduced to XV.HCl, hygroscopic needles, and XV, decompose from 160°, liberated by NaHCO3 treatment.

IT 109247-43-0P, Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl-  
RL: PREP (Preparation)  
(preparation of)  
RN 109247-43-0 CAPLUS  
CN Phenol, 2,2'-(iminodimethylene)bis[3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 1959:94827 CAPLUS  
DN 53:94827  
OREF 53:17141d-h

TI The substitution of Mannich groups on some halogenated phenols

AU Berger, Jerry E.; Byrd, David S., Jr.; Meadow, J. R.

CS Univ. of Kentucky, Lexington

SO Trans. Kentucky Acad. Sci. (1958), 19, 77-82

DT Journal

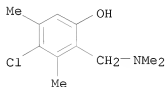
LA Unavailable

AB Mono- and di-Mannich bases of several halogenated phenols were prepared in 75-95% yields. A mixture of 9.36 g. 3,5-dimethyl-4-chlorophenol (I), 4.4 g. pyrrolidine, and 15 ml. absolute EtOH was cooled in ice and treated with 5.4 g. 37% HCHO to give 82.5% 2-(2-pyrrolidinyl)methyl-3,5-dimethyl-4-chlorophenol, m. 44-5° (EtOH), which with HCHO and pyrrolidine gave



88.8% 2,6-bis(2-pyrrolidinyl)methyl-3,5-dimethyl-4-chlorophenol, m. 103.5-4.5°. In similar reactions of other halogenated phenols and secondary amines with HCHO the following Mannich bases were prepared (phenol, Mannich substituent group ortho to the OH, and m.p. given): 6-chlorothymol (II), Me<sub>2</sub>NCH<sub>2</sub>, 54.5-5.5°; II, Et<sub>2</sub>NCH<sub>2</sub>, 26-7°; II, morpholinomethyl, 88-9°; II, N-methylpiperazinomethyl, 87-7.5°; II, piperidinomethyl, 85-6.5°; II, 1-pyrrolidinylmethyl, 58-9°; I, 2-Me<sub>2</sub>NCH<sub>2</sub>, 63-4°; I, 2,6-(Me<sub>2</sub>NCH<sub>2</sub>)<sub>2</sub>, 41-3° (probably a mixture); I, 2-morpholinomethyl, 127-8°; I, 2,6-dimorpholinomethyl, 174-6°; I, 4-methyl-1-piperazinylmethyl, 132-2.5°; I, piperidinomethyl, 148.5-9°; 4-bromophenol, piperidinomethyl, 60-2.5°; 4-bromophenol, 1-pyrrolidinylmethyl, 75-6°; 4-chlorophenol, 1-pyrrolidinylmethyl, 69-71°; 2,4-dichlorophenol (III), Me<sub>2</sub>NCH<sub>2</sub>, 60.5-1.5°; III, morpholinomethyl, 91.5-2°; III, piperidinomethyl, 80.5-1°; III, 1-pyrrolidinylmethyl, 46.5-7.5°; 2,4,5-trichlorophenol (IV), Et<sub>2</sub>NCH<sub>2</sub>, 81-2.5°; IV, morpholinomethyl, 138.5-9.5°; IV, 4-methyl-1-piperazinomethyl, 88-9°; IV, piperidinomethyl, 110-11.5°; IV, 1-pyrrolidinylmethyl, 80-2°

IT 99980-84-4P, Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 99980-84-4 CAPLUS  
 CN Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl- (6CI) (CA INDEX NAME)



L4 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1958:55740 CAPLUS

DN 52:55740

OREF 52:9992b-g

TI Series of o-dimethylaminoalkylphenols

AU Brown, J. P.; McCall, E. B.

CS Monsanto Chem. Ltd., Wrexham, N. Wales

SO Journal of the Chemical Society (1957) 3875-80

CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

OS CASREACT 52:55740

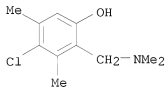
AB 4,3,5-ClMe<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OH (I) with aqueous CH<sub>2</sub>O and Me<sub>2</sub>NH gave 4,3,5,2-ClMe<sub>2</sub>(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>HOH (II), m. 65-6° (MeOH). 4,3,5-ClMe<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OME (III), CH<sub>2</sub>O, and 32% HCl gave 4,3,5,2-ClMe<sub>2</sub>(ClCH<sub>2</sub>)C<sub>6</sub>HOMe (IV), m. 91-2°. IV and NaCN gave the cyanide, m. 120-22°, which was hydrolyzed to 4,3,5,2-ClMe<sub>2</sub>(HO<sub>2</sub>CCH<sub>2</sub>)C<sub>6</sub>HOMe, m. 164-6°. This with SOCl<sub>2</sub> and then Me<sub>2</sub>NH gave the N,N-dimethylamide, m. 130-1°, reduced by LiAlH<sub>4</sub> to 4,3,5,2-ClMe<sub>2</sub>(Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>)C<sub>6</sub>HOH (V), m. 130-2°. Similarly prepared (m.p.s. given) were 4,3,5,2-ClMe<sub>2</sub>(Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>)C<sub>6</sub>HOH (VI), 100-2°, from the N,N-dimethylamide, 104-5°, of

4,3,5,2-ClMe2(HO2CCH2CH2)C6HOME (VII), 116-17°, and 4,3,5,2-ClMe2(Me2N(CH2)4)C6HOH (VIII), 159-60°, from the N,N-dimethylamide, 83-6°, of 4,3,5,2-ClMe2[HO2C(CH2)3]C6HOME (IX), 117-18°. VII was obtained by malonic ester synthesis from IV; 2,3,5,4-ClMe2[(HO2C)2CHCH2]C6HOME m. 166-8°; di-Et ester, m. 77-8°. IX resulted from Clemmensen reduction of 4,3,5,2-ClMe2[HO2C(CH2)2CO]C6HOME, m. 178-81°, prepared from III, (CH2CO)2O, and AlCl3. I and ClCH2COC1 (X) gave the chloroacetate, m. 50-2°, which on heating with AlCl3 cyclized to 5-chloro-4,6-dimethylcoumaranone, m. 137-40°. Similarly I and Cl(CH2)2COC1 gave the  $\beta$ -chloropropionate, m. 51-2°, which cyclized to 6-chloro-5,7-dimethylchromanone, m. 70-1° (2,4-dinitrophenylhydrazone m. 265°), identical with the product prepared by H2SO4 treatment of 4,3,5-ClMe2C6H2O(CH2)2CO2Et (XI), m. 46-9°. XI resulted from the reaction of CH2:CHCO2Et with I in the presence of the Na salt of I. III, X, and AlCl3 gave 4,3,5,2-ClMe2(ClCH2CO)C6HOME, m. 133-5°, converted with Me2NH to 4,3,5,2-ClMe2(Me2NCH2CO)C6HOME; hydrochloride m. 210-25°. An attempted azlactone synthesis from 4,3,5,2-ClMe2(HCO)C6HOH gave 3-acetamido-6-chloro-5,7-dimethylcoumarin, subliming above 300°. III, HCONMePh, and POCl3 gave a little 4,3,5,2-ClMe2(HCO)C6HOME, m. 106-7°. Also prepared were (m.ps. given): the OH analog (XII), 145-50°, of IX; the dimethylamide, 182-3°, of XII, which with LiAlH4 gave VIII; 3,5,2-Me2[HO2C(CH2)3]C6H2OH (XIII), 130-32°, from IX with 66% HI; the dimethylamide, 179-81°, of XIII; the Me ester (XIV), 41°, of IX; 4,3,5,2-ClMe2[HO(CH2)4]C6HOME (XV), 61°, from XIV with LiAlH4; p-nitrobenzoate, 89-91°, of XV; 4,3,5,2-ClMe2[Br(CH2)4]3,5-Me2C6HOME, 124°, from XV and 48% HBr; quaternary salt, 186-90°, from C5H5N.HCl and XV; 4,3,5,2-ClMe2[HO(CH2)4]C6HOH, 105-6°, from XII and LiAlH4. In vitro II, V, VI, VIII and their quaternary salts showed poor to moderate antibacterial activity, increasing with the length of the alkyl group, against *Bacillus mycoides*, *Staphylococcus aureus*, and *Escherichia coli*.

IT 99980-84-4P, Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl-  
RL: PREP (Preparation)  
(preparation of)

RN 99980-84-4 CAPLUS

CN Phenol, 4-chloro-2-(dimethylaminomethyl)-3,5-dimethyl- (6CI) (CA INDEX NAME)

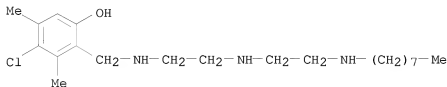


L4 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 1957:69146 CAPLUS  
DN 51:69146  
OREF 51:12516h-i,12517a,12518a  
TI Cleaning, foaming, and wetting agents  
IN Hirschmann, Alexandre  
PA Etablissements Fournier-Ferrier  
DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1007215		19520505	FR	
AB	<p>Good wool-cleaning agents as well as wetting and foaming agents, containing in the same aromatic mol. an amide linkage and a polyoxyethylene group of the general formula <math>\text{RCOHNHR}'\text{ArR}''(\text{OCH}_2\text{CH}_2)_n\text{OH}</math>, where R is a fatty-acid radical, R' and R'' are aliphatic chains, Ar is a substituted mono- or polynuclear aromatic compound, and n is 4-16 or more, are prepared by condensation of at least 3 moles ethylene oxide with fatty amides, derived from &gt;C6 fatty acids and from aromatic hydroxy-containing amines. These amides are represented by the general formula <math>\text{RCONHR}'\text{ArR}''\text{OH}</math>, <math>\text{RCONHArR}'\text{OH}</math>, <math>\text{RCONHR}'\text{ArOH}</math>, and <math>\text{RCONHArOH}</math>. Acid chlorides, prepared by the action of PC13 on coconut-oil fatty acids (I), are condensed with p-aminophenol at 60-80°. The product thus obtained is condensed with 8-12 moles of ethylene oxide, giving products of the general formula <math>\text{RCONHC}_6\text{H}_4(\text{OCH}_2\text{CH}_2)_n\text{OH}</math>, where n = 8-12. Oleic acid is condensed with p-aminobenzyl alc. and the reaction product is condensed with 12-16 moles of ethylene oxide to give the p-(methylenepolyglycoether)-oleylanilide. By condensation of I with p-aminophenylethyl alc. and 12-15 moles ethylene oxide, a product of the general formula <math>\text{RCONHC}_6\text{H}_4\text{CH}_2\text{CH}_2(\text{OCH}_2\text{CH}_2)_n\text{OH}</math> is obtained.</p>				
IT	103508-55-0		(Derived from data in the 6th Collective Formula Index (1957-1961))		
RN	103508-55-0	CAPLUS			
CN	Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)				



L4 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1957:69145 CAPLUS

DN 51:69145

OREF 51:12516g-h

TI Soap compositions

IN Aylesworth, Robert D.

PA Emery Industries, Inc.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2792348		19570514	US 1952-316067	19521021
AB	<p>The drying of soaps is simplified if 0.1% of Na salts of dibasic acids (I) is included with ordinary fatty-acid soaps during manufacture. This permits preparation of soaps of low-titer fatty acids without drying to abnormally low H2O content; preparation of solid soaps with a higher H2O content than normal when employing fatty acids of normal titer, such as tallow or cottonseed acids; and preparation of soap flakes or powders which, for a given H2O</p>				

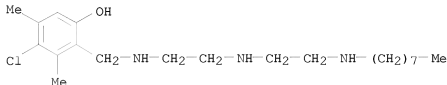
content, are less friable and have less tendency to powder than normal products. The I include malonic, succinic, adipic, azelaic, and sebacic acids.

IT 103508-55-0

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103508-55-0 CAPLUS

CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1957:69141 CAPLUS

DN 51:69141

OREF 51:12515h-i,12516a-b

TI Amphoteric germicidal detergents

PA Th. Goldschmidt A.-G.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 771635		19570403	GB	
	DE 1070189			DE	

AB Compds. having high-bactericidal efficacy, as well as good wetting and detergency, are prepared by treating certain amines with HCHO and phenols. The general formula is:  $C_6H(5-x-y)(RACH_2)_x(R')_yOH$ , where  $x = 1-3$  and  $y = 0-3$ , but  $x + y$  is not greater than 5, R is an alkyl or alkylaryl group having 8-18 C atoms, R' is an alkyl group with 1-3 C atoms, halogen, carboxyl, or  $CH_2(RACH_2)_2(OH)C(CH_3)_2-$ , and A is an amino group such as  $-NR''$ ,  $-NR''(C_2H_4NH)z-$ ,  $-NR''(C_3H_6NH)z-$ , or where R'' is H or an alkyl group with 8-18 C atoms and  $z = 1-3$ . For example, octylamine 25.8, PhOH 1.8, and HCHO 6.0 parts were mixed and, after the exothermic reaction had subsided, the mixture was stirred for 1 hr. at  $100^\circ$ . After cooling, o- and p-(octylaminomethyl)phenol as light-yellow oil was obtained which dissolved to a colloidal solution in alkalies, and to a clear solution in dilute

acids. Analogously, o- and p-(dodecyldiethylenetriaminomethyl)phenyl, 2-(dodecyldiethylenetriaminomethyl)-4-chloro-m-cresol, o-(octyldiethylenetriaminomethyl)-p-cresol, 2-(octyldiethylenetriaminomethyl)-4-chloro-m-xyleneol, o- or p-[p-(dodecylbenzyl)triethylenetetraaminomethyl]phenol, 2,4- or 2,6-bis(tetradecylaminomethyl)phenol, 2,6-bis(octyldiethylenetriaminomethyl)-p-cresol, 2,6-bis(dodecyldiethylenetriaminomethyl)-4-chloro-m-cresol, 3,5-bis(dodecyldiethylenetriaminomethyl)salicylic acid, 2,6-bis(dodecyldiethylenetriaminomethyl)-4-hydroxybenzoic acid, and 2,2-bis[4-hydroxy-3,5-bis(dodecyldiethylenetriaminomethyl)phenyl]propane were prepared

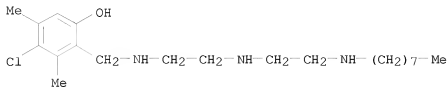
IT 103508-55-0P, Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]-

RL: PREP (Preparation)

(preparation of)

RN 103508-55-0 CAPLUS

CN Phenol, 4-chloro-3,5-dimethyl-2-[[[2-[(2-octylaminoethyl)amino]ethyl]amino]methyl]- (6CI) (CA INDEX NAME)



L4 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1956:12096 CAPLUS

DN 50:12096

OREF 50:2468b-e

TI The structure of artificial resins. II. The action of aromatic amines on dibenzylamines, tribenzylamines, and dibenzyl ethers

AU Zigeuner, G.; Weichsel, H.

CS Univ. Graz, Austria

SO Monatshefte fuer Chemie (1955), 86, 154-64

CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA Unavailable

OS CASREACT 50:12096

AB cf. C.A. 48, 14285b. Cleavage with aromatic amines is employed for the degradation of phenol-(CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub> condensates and related model compds. R<sub>2</sub>NH[R = 2,3,5-HO(Me)C<sub>6</sub>H<sub>2</sub>CH<sub>2</sub>] (I) (0.5 g.), and 1 g. urea, heated 3 h. at 160° gives a 95% yield RNHCONH<sub>2</sub> (II), m. 192°. Treated similarly, R<sub>2</sub>N (III) gives 55% of II. I (0.5 g.) and 1 g. PhNH<sub>2</sub>, heated 2 h. at 160°, gives a 67% yield of PhNHR, m. 87°. Similarly, I and p-MeC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> (IV) gives 63% of RNHC<sub>6</sub>H<sub>4</sub>Me-p (V), m. 98°. III and IV yield 55% of V. R<sub>2</sub>O (VI) (0.5 g.), heated with 1.5 g. urea for 2 h. at 160°, gives a 74% yield of II. VI (0.5 g.) and 1 g. IV heated 1 1/2 h. at 160° gives 73% of V. Other compds. similarly prepared were: 2,3-HO(Me)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NHC<sub>6</sub>H<sub>4</sub>Me-4, m. 76°; 2,3,6-HO(Me)C<sub>6</sub>H<sub>2</sub>CH<sub>2</sub>NHC<sub>6</sub>H<sub>4</sub>Me-4, m. 143°; 2,4,6-HO(Me)C<sub>6</sub>H<sub>2</sub>CH<sub>2</sub>NHC<sub>6</sub>H<sub>4</sub>Me-4, m. 125°; 2,5-HO(Me)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NHC<sub>6</sub>H<sub>4</sub>Me-4, m. 85°; 2,6-bis(p-toluidinomethyl)-4-methylphenol, m. 118°; 2,6-bis(p-toluidinomethyl)-3,5-dimethylphenol, m. 134°; 2,6-bis(p-toluidinomethyl)-4-tert-butylphenol, m. 108.5°; 2,4,6-tris(2-hydroxy-3,5-dimethylbenzyl)-3,5-dimethylphenol, m. 209°; N-(4-hydroxy-3,5-dimethylbenzyl)anthranilic acid, m. 173° (Me ester, m. 115°); N-(4-hydroxy-2,5-dimethylbenzyl)anthranilic acid, m. 186°; N-(2-hydroxy-3,5-dimethylbenzyl)anthranilic acid, m. 165°.

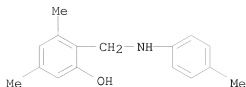
IT 855410-04-7P, Phenol, 3,5-dimethyl-2-p-toluidinomethyl-

RL: PREP (Preparation)

(preparation of)

RN 855410-04-7 CAPLUS

CN Phenol, 3,5-dimethyl-2-[[[4-methylphenyl]amino]methyl]- (CA INDEX NAME)



L4 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1955:75852 CAPLUS

DN 49:75852

OREF 49:14359e-i,14360a-b

TI The synthesis of amphoteric tanning materials. II,III

AU Rosenbusch, K.

CS Tech. Hochschule, Darmstadt, Germany

SO Leder (1955), 6, 80-6

CODEN: LEDEA8; ISSN: 0024-0176

DT Journal

LA Unavailable

AB Aliphatic amines, although more basic than aromatic amines, did not condense with monohydric phenols to amphotans in aqueous solution, but did in organic solvents. In MeOH, equimolar amts. of PhOH, dimethylamine, and HCHO condensed to an acid-soluble oil that was only partly soluble in alkali. The oil was separated to 2 fractions by Et2O-alkali extraction. The main (alkali-insol.) fraction distilled without decomposition at 105-6° under 15 mm. pressure. It was identified as 2-hydroxy-N,N-dimethylbenzylamine by catalytic hydrogenation which gave a quant. yield of 1-methyl-2-cyclohexanol, which formed a 3,5-dinitrobenzoyl ester, m. 97°. It was not a tanning agent because the mol. was too small. Phenolnovolak condensed with dimethylamine in MeOH, to give an amphotan that was soluble in dilute acid and alkali and precipitated at the isoelec. point. The N content

of 9% showed that one dimethylamine group had coupled with each phenolic group. The resin in acid form did not precipitate with gelatin until neutralized to

the quaternary ammonium base stage. The cheaper ethanolamines also condensed with phenolnovolak; the mono compound giving a yellow alc.-insol. resin and the di-compound a resin soluble in alc., acid, or alkali. Catalytic hydrogenation of these resins produced p-cresol-novolak which was readily soluble in alc. or alkali but not in acid. The above condensations occur only in organic solvents, but polyhydric phenols form amphotans in aqueous

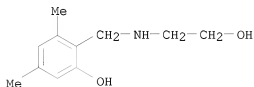
solns Diethanolamine condensed with HCHO to 3-(2-hydroxyethyl)oxazolidine, C5H11O2N, which distilled without decomposition at 128°, 31 mm., decomposed at b.p. 224° and formed a picrate m. 108°. It condensed with resorcinol to N,N-bis(2-hydroxyethyl)-2,4-dihydroxybenzylamine (hydrochloride, colorless needles, m. 145° with decomposition) and with pyrogallol to N,N-bis(2-hydroxyethyl)-3,4,5-trihydroxybenzylamine, m. 145°. These crystalline Mannich bases showed the typical behavior of amphotans. If the precipitate at the isoelec. point was filtered off, its N content approached that of a pure polyhydroxynovolak. Inorg. bases could also be used. NH4Cl, resorcinol, and HCHO, condensed to a tannin that penetrated rapidly because of its small mol. Mannich condensation could also be obtained by fusion. With monohydric phenols the products were soluble, whereas if condensed in aqueous solution they were insol.

Sym-xyleneol,

HCHO, and monoethanolamine condensed to the mono-, di-, or tri-benzylamine

derivative, depending on the amount of amine used. Fusion of phenolnovolak, ethanolamine, and HCHO produced an amphotan similar to that made in alc. solution. Condensation by fusion can also be obtained with polyhydric phenols and amine salts instead of the free base, provided free acid is absent. The most important use for the Mannich condensation in the tanning chemistry lies in the possibility of changing vegetable tannins to amphotannins. A type reaction for a hydrolyzable and a condensed tannin are shown. Exptl. work was reported previously (C.A. 48, 13249e).

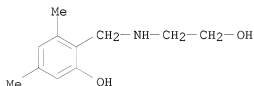
IT 856374-44-2P, Ethanol, 2-(4,6-dimethylsalicylamino)-  
 856374-45-3P, Ethanol, 2-(4,6-dimethylsalicylamino)-, picrate  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 856374-44-2 CAPLUS  
 CN Phenol, 2-[(2-hydroxyethyl)amino]methyl]-3,5-dimethyl- (CA INDEX NAME)



RN 856374-45-3 CAPLUS  
 CN Ethanol, 2-(4,6-dimethylsalicylamino)-, picrate (5CI) (CA INDEX NAME)

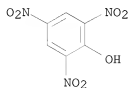
CM 1

CRN 856374-44-2  
 CMF C11 H17 N O2



CM 2

CRN 88-89-1  
 CMF C6 H3 N3 O7

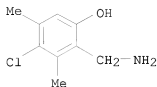


L4 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1952:11359 CAPLUS  
 DN 46:11359  
 OREF 46:2009a-f  
 TI Method for preparing secondary amines and Schiff bases from phenols and hexamine  
 AU Duff, J. C.; Furness, V. I.  
 CS Coll. Technol., Birmingham, UK  
 SO Journal of the Chemical Society (1951) 1512-15  
 CODEN: JCSQA9; ISSN: 0368-1769  
 DT Journal  
 LA Unavailable  
 OS CASREACT 46:11359  
 AB The phenol (10 g.) and 4 g. H3BO3 in 40 mL. EtOCH2CH2OH, treated with 5 g. (CH2)6N4, refluxed 2 h., and poured into H2O, give the following amines; the yield is indicated. Bis(o-hydroxybenzyl)amine, m. 190-200° (decomposition), 2.5 g.; HCl salt; bis(2-hydroxy-3-methylbenzyl)amine, m. 150-5° (decomposition), 5.1 g.; 4-Me isomer, m. 150-7° (decomposition), 7.5 g.; 5-Me isomer, m. 168-70° (decomposition), 7.7 g.; HCl salt. Bis(2-hydroxy-5-chlorobenzyl)amine, m. 155-60°, 2.8 g.; HCl salt. Bis(2-hydroxy-5-chloro-6-methylbenzyl)amine, m. 185-90° (decomposition), 5.5 g.; HCl salt. Bis(2-hydroxy-1-naphthylmethyl)amine, m. 170-8° (decomposition), 6.1 g.; HCl salt. Bis(3-chloro-6-hydroxy-2,4-dimethylbenzyl)amine, m. 219° (decomposition), 6.8 g.; HCl salt. Bis(2-hydroxy-4, 6-dimethylbenzyl)amine, HCl, m. 215-20° (decomposition), 4.5 g. Bis(4-hydroxy-1-naphthylmethyl)amine, pale yellow, m. 205° (decomposition), 4.7 g.; HCl salt. The above amines are not hydrolyzed on boiling in EtOH with HCl. Schiff bases were obtained on heating 5 g. amine and 5 g. (CH2)6N4 in 15 mL. AcOH on the water bath (time and yield given). 2-Hydroxy-N-(2-hydroxybenzylidene)benzylamine (16 h.), bright yellow, 1.2 g.; 2-hydroxy-N-(2-hydroxy-3-methylbenzylidene)-3-methylbenzylamine (9 h.), orange, 3.8 g.; 2-hydroxy-N-(2-hydroxy-4-methylbenzylidene)-4-methylbenzylamine (9 h.), bright yellow, 2.7 g.; 2-hydroxy-N-(2-hydroxy-5-methylbenzylidene)-5-methylbenzylamine (9 h.), bright yellow, 3.5 g.; 5-chloro-2-hydroxy-N-(5-chloro-2-hydroxybenzylidene)benzylamine (6 h.), yellow, 4.2 g.; 3-chloro-6-hydroxy-N-(3-chloro-6-hydroxy-2-methylbenzylidene)-2-methylbenzylamine (6 h.), bright yellow, 3.7 g.; 3-chloro-N-(3-chloro-6-hydroxy-2,4-dimethylbenzylidene)-6-hydroxy-2,4-dimethylbenzylamine (6 h.), orange yellow, 3.7 g.; 2-hydroxy-N-(2-hydroxy-5-phenylbenzylidene)-5-phenylbenzylamine (6 h.), bright yellow, 4.9 g.; 2-hydroxy-N-(2-hydroxy-4,6-dimethylbenzylidene)-4,6-dimethylbenzylamine (2 h.), bright yellow, 2 g.; 4-hydroxy-N-(4-hydroxy-1-naphthylmethylene)-1-naphthylmethylamine (2 h.), yellow, 4.3 g. Hydrolysis of the Schiff bases was carried out by heating 2 g. in 20 mL. of a mixture of equal vols. of EtOH and HCl (d. 1.17) to the b.p. and steam distilling the filtrate. The products are the corresponding aldehyde, the amine, and NH4Cl. 4-Chloro-2-formyl-3-methylphenol, m. 100.5°; 3-chloro-6-hydroxy-2,4-dimethylbenzylamine-H Cl. (PhCH2)2NH (5 g.) and 1 g. (CH2)6N4 in 11 mL. AcOH, boiled 5 min., give 1.2 g. BzH and PhCH2NH2. These reactions are regarded as explaining the mechanism of the general method for preparing o-hydroxyaldehydes described by Duff (C.A. 36, 1597.3).  
 IT 7552-02-2P, Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride 859784-25-1P, 3,5-Xylenol, 2,2'-(iminodimethylene)di-, hydrochloride 859784-27-3P, 3,5-Xylenol, 2,2'-(iminodimethylene)bis[4-chloro-, hydrochloride 859784-30-8P, 3,5-Xylenol, 2,2'-(iminodimethylene)bis[4-chloro-  
 RL: PREP (Preparation)  
 (preparation of)

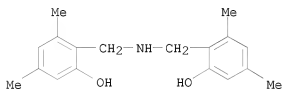


RN 75552-02-2 CAPLUS  
 CN Phenol, 2-(aminomethyl)-4-chloro-3,5-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



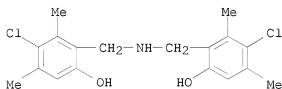
● HCl

RN 859784-25-1 CAPLUS  
 CN 3,5-Xylenol, 2,2'-(iminodimethylene)di-, hydrochloride (5CI) (CA INDEX NAME)



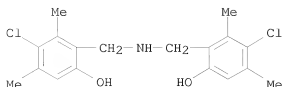
● HCl

RN 859784-27-3 CAPLUS  
 CN Phenol, 4-chloro-2-[[[(3-chloro-6-hydroxy-2,4-dimethylphenyl)methylamino]methyl]-3,5-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 859784-30-8 CAPLUS  
 CN Phenol, 4-chloro-2-[[[(3-chloro-6-hydroxy-2,4-dimethylphenyl)methylamino]methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1951:49820 CAPLUS

DN 45:49820

OREF 45:8475d-f

TI Formaldehyde condensations with phenol and its homologs. XI. The preparation of 2-hydroxymethyl-3,5-dimethylphenol by a new general method

AU Finn, S. R.; Musty, J. W. G.

SO Journal of Applied Chemistry (1951), 1, 182-4

CODEN: JACHAU; ISSN: 0021-8871

DT Journal

LA Unavailable

AB cf. C.A. 45, 7074e. 3,5-Xylenol (I) with HCHO (II) forms substances other than 2-methylol-3,5-xylenol (III) (cf. C.A. 45, 1537). The diacetate (IV), b0.5 152-3°, n20D 1.5040°, of III resulted in 11 g. yield by refluxing 10 g. 2-(dimethylaminomethyl)-3,5-xylenol (V) 6 hrs. with 15 ml. Ac2O and also from III with Ac2O and K2CO3 but not with Ac2O and H2SO4. 2,4,6-Me2(HO)C6H2CHO (5.7 g.) in dry Et2O was added gradually to 1.1 g. LiAlH4 and Et2O, the mixture poured after 20 min. into cold H2O, allowed to stand 24 hrs. with addition of HOAc to maintain acidity, neutralized, filtered to remove inorg. solids, and the solution was concentrated in

vacuo to 0.2 volume and cooled to give 1.67 g. solid, m. 60-6°.

Recrystn. from petr. ether-C6H6 gave III, m. 88°. A similar reduction of IV (10.2 g.) with 3 g. LiAlH4 gave 1 g. III. The synthesis of III by way of V is according to the new general method (C.A. 45, 61681). The phenylurethan of III m. 171°.

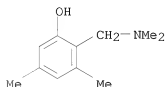
IT 63487-28-5P, Phenol, 2-(dimethylaminomethyl)-3,5-dimethyl-

RL: PREP (Preparation)

(preparation of)

RN 63487-28-5 CAPLUS

CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1947:2215 CAPLUS

DN 41:2215

OREF 41:414c-i,415a-i,416a-i

TI Aminoalkylphenols as antimalarials. I. Simply substituted α-aminocresols

AU Burckhalter, J. H.; Tendick, F. H.; Jones, Eldon M.; Holcomb, W. F.;

CS Rawlins, A. L.  
SO Parke, Davis Co., Detroit, MI  
SO Journal of the American Chemical Society (1946), 68, 1894-1901  
CODEN: JACSAT; ISSN: 0002-7863  
DT Journal  
LA Unavailable  
AB

In this paper Q-B4 indicates the quinine equivalent of the compound against *P. gallinaceum* in chicks, Q-D1 against *P. lophurae* in ducks, and Q-D2 and Q-J1 against *P. cathemerium* in ducks and canaries, resp. A value of 0.2 represents the activity of a drug that is 20% as effective as quinine; 0.2i indicates that the drug is inactive at 5 times the ED of quinine, and 0.2t indicates that at 0.2i the drug is toxic. The fact that 4,2-Me3CCH2CMe2(Me2NCH2)C6H3OH (I) (SN 5018) (U.S. 2,033,092, C.A. 30, 2669.2) was found to have Q-B4 0.3 and Q-J1 0.67i led to the synthesis of several hundred derivs. of o-H2NC6H4OH, of which 109 new compds. (and pharmacol. tests on 19 others) are reported in the present paper. The compds. were prepared by the Mannich reaction, in which phenols with at least one open position ortho or para to a phenolic HO group were treated with HCHO and aliphatic amines; (HCHO)3 and 37% HCHO were equally useful in the reaction. An equimol. mixture of the amine and HCHO in sufficient EtOH to give a clear solution on heating is added (after cooling) to the phenol in EtOH (solution or suspension), the mixture allowed to stand 1 h., refluxed 2 h., the solution concentrated, extracted with ether, and the substituted amine isolated

as such or as the HCl(HBr) salt. Various modifications of this procedure are indicated. (AcCH2)2 (57 g.), 54.5 g. p-H2NC6H4OH, 100 cc. absolute EtOH, and 1 cc. AcOH, refluxed 20 h., give 82% 4-(2,5-dimethyl-1-pyrrolyl)phenol, m. 104-6° (not analyzed because of discoloration in air and light). (4-HOC6H4)2O (preparation in 40% yield given) (20.2 g.), 27.8 g. K2CO3, and 150 cc. Me2CO, heated to boiling, treated with 24.2 g. CH2CHCH2Br during 30 min., the mixture refluxed 2 h., and the resulting allyl ether heated at 250°/20 mm., give 52% 3,3'-diallyl-4,4'-oxybiphenol, bl.5 195-200°. 2-Allyl-4-tert-butylphenol, b8 127-9°, 79%. The MeCl derivative of I (SN 7867) has Q-B4 0.3i. The following derivs. of 4-(1,1,3,3-tetramethylbutyl)-o-cresol were prepared: α-diamylamino (SN 7494), whose HBr salt m. 143°, 81%, Q-B4 0.05i; α-1-piperidyl (SN 6798), m. 70°, 95%, Q-B4 0.02; α-4-morpholinyl-HCl (SN 7137), m. 200°, 52%, Q-B4 0.03i; α-[ethyl(2-hydroxyethyl)amino]-HCl (SN 7821), m. 151°, 93%, Q-B4 0.08; α-[bis(2-hydroxyethyl)amino] (SN 6803), m. 81°, 24%, Q-B4 0.03; α-dibenzylamino (SN 6797), m. 118°, 70%, Q-B4 0.02i; 6-methyl-α-dimethylamino (SN 6804), Q-B4 0.20; 6-chloro-α-diethylamino (SN 7491), Q-B4 0.11. Derivs. of α-dimethylamino-o-cresol, (SN 7502), Q-B4 0.03i, prepared were: 6-Me (SN 7498), Q-B4 0.03i, Q-J1 0.05i; 4-tert-Bu (HCl salt) (SN 7497), Q-B4 0.1. α-Diethylamino-o-cresol (II) (SN 4769) b3 100-10° (HCl salt, m. 135°, 32%, Q-J1 0.2i). Derivs. of II: 6-Me, b3 107-8° (HCl salt, m. 161°, 36%, Q-B4 0.05t; 4-Me (SN 6805), b4 122, 71%, Q-B4 0.04 (HCl salt, m. 157°, Q-J1 0.05i); 4-tert-Bu (SN 7496), m. 36°, 38%, Q-B4 0.4; 4-tert-butyl-6-hydroxy (SN 7741), m. 142°, 96%, Q-B4 0.07i; 4-(2-methylcyclohexyl) (HCl salt) (SN 7503), m. 148°, 46%, Q-B4 0.18t; 6-heptyl (HCl salt) (SN 8459), m. 126°, 46%, Q-B4 0.1; 4-octyl (HCl salt) (SN 8458), m. 86°, 39%, Q-B4 0.04i; 4-dodecyl (SN 7500), Q-B4 0.10; 4-Cl (HCl salt) (SN 7493), m. 158°, 56%, Q-B4 0.06; 4-Br (HCl salt) (SN 7488), m. 165°, Q-B4 0.06; 6-Br (HCl salt) (SN 7296), m. 175°, 10%, Q-B4 0.05i; 4-methyl-6-bromo (HCl salt) (SN 13,700), m. 170°, 65%, Q-B4 0.05i; 4-bromo-6-Me (HCl salt) (SN 8456), m. 175°, 38%, Q-B4 0.4t; 6-cyclohexyl-6-bromo (SN

9000), m. 92°, 63%, Q-B4 0.06; 4-chloro-6-(3-buten-2-yl) (HCl salt) (SN 8294), m. 130°, 44%, Q-J1 1.0; 4-tert-amyl-6-chloro (HCl salt) (SN 7492), m. 148°, 83%, Q-B4 0.1; 4-chloro-5-Me (HCl salt) (SN 8497), m. 192°, 51%, Q-B4 0.08; 3-methyl-4-chloro-6-hexyl (HCl salt) (SN 8370), m. 132°, 81%, Q-B4 0.06; 4,5-di-Me (HCl salt) (SN 7304), m. 190°, 83%, Q-B4 0.2t; 3,5-di-Me (HCl salt) (SN 10,989), m. 156°, 77%, Q-B4 0.25; 3,5,6-tri-Me (HCl salt) (SN 7303), m. 175°, 94%, Q-B4 0.10, Q-J1 0.4t; 4-tert-butyl-5-Me (HCl salt) (SN 10,505), m. 177°, 12%, Q-B4 0.05i; 4-tert-butyl-6-Me (HCl salt) (SN 9576), m. 150°, 45%, Q-B4 0.3, Q-J1 1.0; 4-tert-butyl-6-allyl (HCl salt) (SN 7819), m. 139°, 48%, Q-B4 0.2; 4-tert-amyl-6-allyl (HCl salt) (SN 8051), m. 151°, 41%, Q-B4 0.17; 4-cyclohexyl-6-allyl (HCl salt) (SN 8383), m. 142°, 59%, Q-B4 0.18; 4-tert-butyl-6-cyclohexyl (HCl salt) (SN 8393), m. 192°, 56%, Q-B4 2.0. 4-Chloro- $\alpha$ -(1-piperidyl)-o-cresol (SN 6799) m. 57°, 82%, Q-B4 0.04i; 5-Me derivative (SN 7298), m. 85°, 62%, Q-B4 0.08i. 4-Chloro-5-methyl- $\alpha$ -(4-morpholinyl)-o-cresol (HCl salt) (SN 6796) m. 215°, 31%, Q-B4 0.05i. 4-PhC6H4OH (17 g.), 18 g. C6H4(CO)2NCH2OH, 200 cc. benzene, and 6 drops concentrated H2SO4, refluxed 2 h., evaporated to dryness, the residue in

100

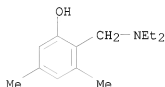
cc. alc. refluxed 20 min. with 10 cc. 85% N2H4.H2O and then 1 h. with 200 cc. 3 N HCl, give 29% 4-phenyl- $\alpha$ -amino-o-cresol (III), light tan, m. 157-8° (HCl salt (SN 9578), m. 235°, Q-J1 1.0). Analogs of III:  $\alpha$ -dimethylamino (SN 5017), Q-B4 0.2, Q-J1 1.0, Q-D1 0.12, Q-D2 0.25;  $\alpha$ -diethylamino (HCl salt) (SN 7301), m. 165°, 46%, Q-B4 0.12i;  $\alpha$ -[ethyl(2-hydroxyethyl)amino] (HCl salt) (SN 7487), m. 149°, 18%, Q-B4 0.03i;  $\alpha$ -(1-piperidyl) (SN 7142), m. 90°, 62%, Q-B4 0.02;  $\alpha$ -(4-morpholinyl) (SN 7143), Q-B4 0.03i; 6-hydroxy- $\alpha$ -diethylamino (SN 7740), m. 108°, 64%, Q-B4 0.05i, Q-J1 0.2t. 5-Phenyl- $\alpha$ -diethylamino-o-cresol (SN 7820) m. 78°, 76%, Q-B4 0.4, Q-J1 0.4t; 6-Ph isomer (SN 6895), Q-B4 0.2. 6-Phenyl- $\alpha$ -ethylamino-o-cresol (SN 9283) m. 186°, Q-B4 0.2;  $\alpha$ -(2-hydroxyethyl)amino derivative (SN 8268), Q-B4 0.1, Q-D1 0.06, Q-D2 0.25;  $\alpha$ -decylamino derivative (HCl salt) (SN 8298), m. 134°, 50%, Q-B4 0.13. 4-Phenyl-6-chloro- $\alpha$ -diethylamino-o-cresol-HCl m. 141°, 31%, Q-J1 0.17;  $\alpha$ -1-piperidyl analog (free base) (SN 7489), m. 80°, 92%, Q-B4 0.1i. 4-Phenyl-6-bromo- $\alpha$ -diethylamino-o-cresol-HCl (SN 7294) m. 141°, 89%, Q-B4 0.5i. 4-Chloro-6-phenyl- $\alpha$ -diethylamino-o-cresol-HCl (SN 7297), m. 128°, 43%, Q-B4 0.18, Q-D1 0.5, Q-D2 1.0, Q-J1 1.0; 4-Br analog (SN 14,111), m. 146°, 70%, Q-B4 0.3. 2-Chloro-3-phenyl- $\alpha$ -diethylamino-o-cresol (SN 7490), m. 65°, 54%, Q-B4 0.2. 4-tert-Butyl-6-phenyl- $\alpha$ -dimethylamino-o-cresol-HCl (SN 7282) m. 207°, 85%, Q-B4 1.5, Q-J1 2.0;  $\alpha$ -diethylamino analog (SN 7744), m. 173°, 83%, Q-B4 2.0, Q-D1 2.0, Q-J1 1.0i [O-Ac derivative (SN 9636), m. 201°, 67%, Q-B4 1.5; O-Me derivative (SN 10,122), m. 142°, 50%, Q-B4 0.16t; the latter was prepared from 4-tert-butyl-6-phenylanisole (b3 43-5°) through the 2-Br derivative (b2 147-8°) and its Grignard reagent];  $\alpha$ -ethylamino analog (SN 9557), m. 216°, 42%, Q-B4 2.5;  $\alpha$ -(2-hydroxyethyl)-amino analog, with 2 mols. H2O (SN 9202), m. 158°, 45%, Q-B4 1.0. 4-tert-Amyl-6-phenyl- $\alpha$ -diethylamino-o-cresol-HCl (SN 8368), m. 168°, 80%, Q-B4 1.6, Q-D1 1.0, Q-J1 2.0. 4-(1,1,3,3-Tetramethylbutyl)-6-phenyl- $\alpha$ -diethylamino-o-cresol-HCl (SN 8303) m. 178°, 88%, Q-B4 0.6, Q-D1 1.0, Q-J1 0.2. 4-Phenyl-6-(3-buten-2-yl)- $\alpha$ -diethylamino-o-cresol-HCl (SN 8289) m. 151°, 50%, Q-D4 0.55. 4-tert-Butyl-5-phenyl- $\alpha$ -diethylamino-o-cresol-HCl (SN 8500) m. 190°, 83%, Q-B4 0.08. 4-Benzyl- $\alpha$ -diethylamino-o-cresol-HCl (SN

7499) m. 160°, 10%, Q-B4 0.13, Q-D1 0.06; 6-isomer (SN 7300) m. 149°, 48%, Q-B4 0.06, Q-D1 0.09; 4,6-dibenzyl analog (SN 14,309), m. 152°, Q-B4 0.06; 4-benzyl-6-Me analog (free base) (SN 7742), m. 106°, 59%, Q-B4 0.12t; 4-(1-methyl-1-phenylethyl) analog (SN 8049), m. 150°, 42%, Q-B4 0.05i; 4-(1-methyl-1-phenylethyl)-6-hydroxy analog (free base) (SN 8996), m. 97°, 35%, Q-B4 0.1t.

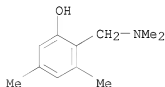
4-Substituted  $\alpha$ -diethylamino-o-cresols: MeO (SN 7363), b3 133-5°, 52%, Q-B4 0.08i, Q-J1 0.4t; EtO (SN 7364), slightly greenish liquid, b3 144-7°, 66%, Q-B4 0.06i, Q-J1 0.4; benzyloxy (HCl salt) (SN 8371), m. 133°, 37%, Q-B4 0.04; phenoxy (HCl salt) (SN 8048), m. 130°, 39%, Q-B4 0.04, Q-J1 1.0i; 2,5-dimethyl-1-pyrryl, m. 164°, 25%, Q-B4 0.5i; 4-morpholinyl (HCl salt) (SN 8309), m. 176°, Q-B4 0.15; cyano (HCl salt) (SN 7738), m. 208°, 37%, Q-B4 0.05; the CN derivative with dry HCl in absolute EtOH gives the imido ester

di-HCl salt, m. 167-9° (decomposition); shaken with EtOH-NH3, this gives 68% of the guanyl derivative (di-HCl salt) (SN 7637), m. 215°, Q-B4 0.05i. 2-Diethylaminomethyl-1-naphthol-HCl (SN 7299), m. 150°, 57%, Q-B4 0.1; 1-diethylaminomethyl-2-naphthol-HCl (SN 6806), m. 164°, 78%, Q-J1 0.1t; 7-dimethylaminomethyl-8-quinolinol-HCl, m. 186°, 74%, Q-B4 0.05i, Q-J1 0.33t; 7-(1-piperidylmethyl)-8-quinolinol, m. 194°, 52%, Q-B4 0.11; 8-diethylaminomethyl-7-quinolinol, m. 220°, 37%, Q-J1 0.33t.  $\alpha, \alpha'$ -Bis derivs. of 4,4'-bi-o-cresols (di-HCl salts): diethylamino (SN 6894), m. 225°, 55%, Q-B4 0.17t, Q-J1 0.5i; 6,6'-dimethyl derivative (SN 7824), m. 215°, 64%, Q-B4 0.75; 6,6'-di-Pr derivative (SN 7827), m. 221°, 70%, Q-B4 1.0; 6,6'-bis(2-chloroallyl) derivative, m. 208°, 34%, Q-B4 2.5; 6,6'-bis(methallyl) derivative (SN 8379), m. 263°, 17%, Q-B4 0.11t;  $\alpha, \alpha'$ -bis (diethylamino)-5,5'-bi-o-cresol (SN 10,271), m. 106°, 92%, Q-B4 4.0.  $\alpha, \alpha'$ -Bis derivs. of 6,6'-diallyl-4,4'-bi-o-cresol (di-HCl salts): dimethylamino (SN 8316), m. 241°, 47%, Q-B4 4.0; diethylamino (SN 6771), m. 209°, 67%, Q-B4 2.0, Q-J1 0.5; dipropylamino (SN 8315), m. 187°, 38%, Q-B4 1.0, Q-J1 0.5; dibutylamino (SN 8380), m. 178°, 57%, Q-B4 0.25; 1-piperidyl (SN 9558), m. 250°, 78%, Q-B4 0.5; 4-morpholinyl (SN 10,150), m. 251°, 70%, Q-B4 0.05; (2-hydroxyethylamino) (SN 9187), m. 111°, 24%, Q-B4 0.6; [bis(2-hydroxyethyl)amino] (SN 9188) m. 130°, 20%, Q-B4 0.06; O,O'-diacetyl- $\alpha, \alpha'$ -bis(diethylamino) derivative (SN 9635), m. 224°, 90%, Q-B4 1.3; O,O'-dipropionyl derivative (SN 11,000), m. 185°, 30%, Q-B4 0.8. 4,4'-Oxybis( $\alpha$ -diethylamino-o-cresol) (SN 5918) m. 99°, 66%, Q-B4 1.0; bis-6-allyl derivative (di-HCl salt) (SN 8450), m. 240°, 47%, Q-B4 0.21. 4,4'-Isopropylidenebis(6-methyl- $\alpha$ -diethylamino-o-cresol)-2HCl (SN 7737) m. 210°, 48%, Q-B4 0.09; bis-6-Ph analog (free base) (SN 9186), m. 75°, 77%, Q-B4 0.5. 4,4'-(1,2-Diethyl-1,2-dihydroxy-ethylene)bis( $\alpha$ -diethylamino-o-cresol) (SN 7828) m. 153°, 23%, Q-B4 0.2. 4,4'-(1,2-Diethylvinylene)bis( $\alpha$ -diethylamino-o-cresol) (SN 7826) m. 110°, 50%, Q-B4 0.4. 4,4',4'',4'''-(Ethylenediethylidene) tetrakis ( $\alpha$ -diethylamino-o-cresol) (SN 8583) m. 150°, 6% Q-B4 1.4.  $\alpha$ -Diethylamino-p-cresols: 3,6-di-Me (SN 8999), m. 104°, 20%, Q-B4 0.04i; 3-methyl-6-iso-Pr (SN 9001), m. 93°, Q-B4 0.05; 2-Ph (SN 6772), Q-B4 1.2, Q-D1 0.13, Q-J1 2.0; 2-chloro-6-Ph (HCl salt) (SN 8050), m. 162°, 80%, Q-B4 0.4, Q-D1 0.5i; 2-allyl-6-Ph (HCl salt) (SN 8388), m. 128°, 66%, Q-B4 0.4, Q-D1 0.25t; 2,6-di-Ph (HCl salt) (SN 10,210), m. 189°, 57%, Q-B4 0.12, Q-J1 1.0i. 2,4-Bis(diethylaminomethyl)-6-cyclohexylphenol-2HCl (SN 7736), m. 199°, Q-B4 0.25; 6-phenylphenol analog (2HCl) (SN 7358), m.

207°, 95%, Q-B4 1.3, Q-J1 0.5; 2,5-bis(diethylaminomethyl)hydroquinone (SN 7356), m. 107°, 62%, Q-B4 0.23.  
 IT 38942-39-1, Phenol, 2-(diethylaminomethyl)-3,5-dimethyl-  
 (hydrochlorides)  
 RN 38942-39-1 CAPLUS  
 CN Phenol, 2-[(diethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



L4 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1939:29791 CAPLUS  
 DN 33:29791  
 OREF 33:4214e-g  
 TI Nuclear methylation of phenols. A new synthesis of intermediates in the preparation of antisterility factors  
 AU Caldwell, Wm. T.; Thompson, Thomas R.  
 SO Journal of the American Chemical Society (1939), 61, 765-7  
 CODEN: JACSAT; ISSN: 0002-7863  
 DT Journal  
 LA Unavailable  
 OS CASREACT 33:29791  
 AB One mole of 3,5-MeC6H3OH, treated with 1 mol 35% aqueous Me2NH and then at a temperature of 25-35° with 1 mol of HCHO, gives 60 g. of 2-(dimethylaminomethyl)-3,5-dimethylphenol, m. 42-2.5°; hydrogenation in dioxane with Cu chromite at 177 atmospheric and 165° for 4 h. gives 58.5% of 2,3,5-Me3C6H2OH. Coupling with p-NaSO3C6H4N2X, reducing the azo dye with Na2S2O4, oxidizing the aminophenol with FeCl3 and reducing the quinone with Na2S2O4 give 27% of 2,3,5-trimethylhydroquinone. C6H6O2 with Me2NH and HCHO gives an almost quant. yield of 2,5-bis(dimethylaminomethyl)hydroquinone, m. 190°; reduction gives 23% of 2,5-dimethylhydroquinone.  
 IT 63487-28-5P, Isopseudocumenol, α2-dimethylamino-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 63487-28-5 CAPLUS  
 CN Phenol, 2-[(dimethylamino)methyl]-3,5-dimethyl- (CA INDEX NAME)



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CA SUBSCRIBER PRICE	-29.60	-29.60

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